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A method for performing restrained dynamics docking of one or multiple substrates on multi-specific enzymes

The present invention relates to a method for performing restrained dynamics docking of one or several substrates having allosteric or synergistic effect on enzymes presenting multispecific and flexible active site. It also concerns a method for determining the 3D-structure of active sites that are flexible and can adapt to different substrates, which is the case for multispecific enzymes such as cytochrome P450.

As of today, various computer graphics systems allow to generate molecular models of large molecules such as proteins from the PDB structural data obtained using X-ray crystallography and NMR. We can cite for example MODELLER, COMPOSER, MATCHMAKER (Tripos), or 3D graphical environments for molecular modeling such as SYBYL (Tripos) or INSIGHT II (Accelrys).

Substrates as well as inhibitors or agonists often act by binding to particular regions of an enzyme or receptor referred as the active site. In industry, the purpose of using these 3D models is to assess the main features of the molecules which are involved in the binding to the active site. New molecules that fit the active site can be designed.

Biological interactions are not possible without flexibility and motion. One of the principal tools in the theoretical study of motion in biological molecules is the method of molecular dynamics simulations (MD). This computational method calculates the time dependent behavior of a molecular system (Karplus and McCammon, 2002). MD simulations have provided detailed information on the fluctuations and conformational changes of proteins and nucleic acids. These methods are now routinely used to investigate the structure, dynamics and thermodynamics of biological molecules and their complexes. They are also used in the determination of structures from x-ray crystallography and from NMR experiments. The molecular dynamics simulations can be used to recreate the successive events in the binding process of a molecule, and thermodynamic parameters implicated in such process can therefore be derived, which is of great interest in the design of active molecules.

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Nevertheless, the methods proposed in the art are based on a relatively low level of calculations of few parameters. It relies only on the molecule energy constrained with a fixed geometry. It relies only on the interaction energy between the molecule and the active site frozen in a fixed geometry.

5 Consequently, there is a need for a model replicating *in silico* the natural process of molecular interactions.

The method according to the invention provides both minimizations and molecular dynamics calculations. More specifically, it provides a new approach which is more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained restrained dynamics docking". This technique employs constrained dynamics simulations, where the only constraints are active sitesubstrate distances.

For example, to explain and predict drug metabolism in organisms, in which the cytochrome P450 (CYP) superfamily of haem-thiolate enzymes plays a central role, it is of large interest to dispose of a molecular picture of the binding sites responsible for the biotransformation. Efficiency of the prediction is then directly related to the molecular precision of the model, which resolution must be obtained at the atomic level to exploit the model for further docking studies.

In mammalian, hepatic cytochrome P450s constitute the major enzymes involved in the metabolism of exogenic compounds. Among them, isozymes of the CYP3 family (such as CYP3A1 and 3A2 in rat, and CYP3A4, CYP3A5, CYP3A7, CYP 3A43 in human) are known to metabolize the majority of drugs in clinical use. These are multi-specific enzymes, able to metabolize a large variety of structurally diverse chemicals or substrates including steroids, linear or cyclized peptides (Delaforge et al. 1997, Delaforge et al. 2001, Aninat et al. 2001), generally fairly lipophilic, within a broad range of molecular sizes from testosterone (Mw 288) to cyclosporin A (Mw 1203).

The inventory of known substrates for CYP 3A contains a large variety of different molecules having apparently no common structural factors. Actually it can be estimated that more than five hundred utilized drugs can be recognized and metabolized by CYP 3A (Guengerich 1995, Wrighton et al. 2000, Lewis 2001). Closer inspection of the precise transformations catalyzed by CYP 3A indicates that there is an important regio- and stereo-selectivity for each substrate. The active site

can accommodate relatively rigid substrates such as aflatoxin derivatives or steroids, that are oxidized almost exclusively at a precise position. Thus CYP 3A4 catalyzes the testosterone oxidation exclusively at the 6β position, whereas CYP 3A7 oxidizes dehydroepiandrosterone (DHEA) or its 3 sulfate conjugate exclusively on the 16α position (see Figures 4A and 4B). In addition to such small substrates, CYP 3A metabolize also large molecules such as cyclosporin A (MW 1202), macrolide antibiotics (MW around 600) or ergot derivatives (MW from 500 to 700).

The recognized substrates can have endogenous origin such as steroids or can be drugs or compounds found in food. For example, grapefruit juice contains bergamottin derivatives having specific CYP 3A inhibitory activities (Schmiedlin-Ren et al. 1997). Linear peptides (Delaforge et al. 2001, Hosea et al. 2000) or cyclized peptides (Delaforge et al. 1997) containing from 2 aminoacids (called diketopiperazine, Delaforge et al. 2001, Aninat et al. 2001) to 11 amino-acids (e.g. cyclosporin) are also recognized.

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Following this wide range substrate recognition, a tentative subclassification was established leading to a multi-site hypothesis (Hosea et al. 2000, Ekins et al. 2003) consisting of at least 2 or 3 binding zones in the active site. This hypothesis has been established on the facts that CYP 3A shows often atypical hyperbolic kinetic constants and is thus unable to reach saturation. In addition, the presence in the active site of a second substrate having a different molecular nature lead to either no modification or increased metabolism of both substrates. Such allosteric effects have been clearly described in the case of simultaneous metabolism of steroids such as testosterone and α -natphtoflavone.

Consequently, any molecular model describing correctly the multiple substrate specificity (that takes into account large variations in molecular size and chemical structures), and substrate cooperativity effects within the active site (when two or more drugs interact), is of considerable scientific and industrial interest. Such a molecular model must be able to rationalize the binding of the diverse known substrates, and the orientations of the molecules in the binding site that account for their known positions of metabolism (such as N-demethylations, benzylic hydroxylations etc.).

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CYP3A4 is considered as the main hepatic form and is found in a wide variety of human organs such as intestine, brain or skin. CYP 3A5 is also present in liver and is the major 3A form present in the kidney. The 3A5 isoform is subject to genetic polymorphism. CYP 3A7 is the major 3A isoform present in the foetus whereas 5 CYP3A43 is mainly located in adult prostate or testis. These isoforms share amino acid identities higher than 70%. (Westlind-Johnsson et al. 2003, Gellner et al. 2001, Koch et al. 2002). It is currently accepted that CYP3A4 is the most active isoform for classical P450 3A substrates whereas recent data (Williams et al. 2002) demonstrate equal or slightly reduced activity for CYP3A5 and a significantly lower metabolism capability for CYP3A7 as compared to CYP3A4. Additionally, differences have been observed in term of oxidative regioselectivity of the CYP3A7 compared to other isoforms. As an example, CYP3A7 metabolizes intensively DHEA and especially its sulfate conjugate derivative whereas CYP3A4 is a poor metabolizer. The oxidation by CYP3A7 occurs mostly in the 16a position of DHEA. In contrast, CYP3A7 metabolizes testosterone in both 6β and 16α position whereas CYP3A4 or 3A5 metabolize it almost exclusively in the 6β position (Inoue et al. 2000).

At the contrary of the P450 3A subfamily, other P450 isoforms have more rigid active site, as suggested by the narrow range of recognized substrates or inhibitors.

These P450 isoforms recognize generally a small number of substrates or inhibitors having in common the same shape (i.e. P450 1A isoforms), or the same charge (i.e. CYP 2B, 2C or 2D isoforms), or the same chemical nature such as steroids (i.e. CYP19 or CYP21 isoforms) or lipids (i.e. CYP 4 family).

As no high-resolution 3D structure of CYP3A is today publicly available, due to continuing difficulties in promoting crystallization of intrinsic membrane proteins or due to an unusual conformational flexibility that would explain how CYP3A can accommodate various substrates, it is necessary to rebuild a 3D model structure, integrating the known biochemical data of CYP3A and the structural data of other members of the CYP superfamily. X-ray crystallographic determinations of several bacterial P450 enzymes in the 1990s (see Table 1 for a summary of structural data) have stimulated numerous attempts in modeling microsomal P450S such as human CYP3A4. The chapter 6 of the book "Guide to Cytochromes P450: structure and function" written by David F.V. Lewis reviews the current status of structural and

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modeling investigations of the P450 family (Lewis 2001). This review was however written just before the release of the first mammalian P450 structure (2C5), still today the only one mammalian template available.

Table 1

CYP isoform crystallized	PDB code (resol.)	Organism	Function	No of residues	Reference
P450 cam (complexed by CO+camphor)	3cpp (1.9 Å)	Pseudomonas Putida	Camphor Monooxygenase	414	(Poulos et al. 1985) (Raag and Poulos 1989)
P450 terp	1cpt (2.3 Å)	Pseudomonas sp.	Alpha-terpineol hydroxylation	412	(Hasemann et al. 1994)
P450 BM3	2hpd (2 Å)	Bacillus megaterium	Fatty acid monooxygenase	471	(Ravichandran et al. 1993)
P450 cryF (6-deoxyerythro -nolide B bound)	loxa (2.1 Å)	Saccharopolyspora erythraea	Erythromycin biosynthesis 6S- hydroxylation of 6- deoxyerythronolide B	403	(Cupp-Vickery and Poulos 1995)
P450 nor	1rom (2 Å)	Fusarium oxysporum (denitrifying fungus)	Nitric Oxide Reductase	403	(Park et al. 1997)
P450 2C5	1dt6 (3 Å)	(membrane-type Mammalian) Rabbit	Progesterone 21- Hydroxylase	473 (487)	(Williams et al. 2000)
P450 CYP119 4-Phenylimidazole Bound	lf4t (1.93 Å)	Sulfobolus Solfactaricus Thermophilic bact.	unknown	368	(Yano et al. 2000)
P450 CYP51 4-Phenylimidazole Bound	1e9x (2.1 Å)	Mycobacterium Tuberculosis	14 α-sterol demethylase	455 (451)	(Podust et al. 2001)

Table 1: the eight X-ray crystal structures of P450s available in 2002: six bacterial, one fungal (P450 nor), one mammalian (CYP2C5). The P450_{cam}, P450_{terp}, P450_{eryF}, P450_{nor} belong to class I P450s enzymes, whereas P450_{BM3} belongs to class II enzymes, like microsomal enzymes CYP2C5 and 3A. P450_{BM3} structure is therefore a priori more relevant to rebuilding a structural model of CYP3A, but since the CYP2C5 X-Ray structure has been released, it became obvious that the structural homology between the other bacterial enzymes and microsomal enzymes was better than expected from the poor homology of primary structure (< 25% identity). Then, the relevance of using class I and class II structures together for rebuilding models of class II P450s was no more questionable. In the two examples described in the present invention, the structural model of human CYP3A4 was rebuilt using the six

first structures listed above, with no preference in the structural alignment, and the structural model of human CYP3A7 was rebuilt using four structures among those listed above with again no preference in the structural alignment, *i.e.* P450_{BM3}, P450 EryF, P450 2C5 and CYP51, one of the last published structural sets. CYP119 was not incorporated into the modeling process.

All the proposed models of CYP3A4 obtained by homology modeling are thus so far based on bacterial crystal structure templates: the first was proposed by Ferenczy and Morris and used the X-ray structure of bacterial P450_{cam} as unique template structure (Ferenczy and Morris 1989). Another model was built later by David F.V. Lewis, using also a unique template structure, the P450_{BM3} structure, which was supposed to be more relevant as a template since this P450 was the only one class II enzyme with known three-dimensional structure (Lewis et al. 1996). A third model, based on a multiple structure template, was built by Szklarz and Halpert, using the four first X-ray crystal structures available P450_{cam}, P450_{terp}, P450_{eryF}, and P450_{BM3}. This four-bacterial template approach strategy is closer to our rebuilding strategy, but was still missing some relevance in the absence of a mammalian template. In our hands, the incorporation of the mammalian 2C5 crystal structure into rebuilding steps of models of cytochrome P450 3A proved to be decisive. Inclusion of 2C5 crystal structure had indeed a profound effect on the structural alignment with the five non-mammalian structures, resulting in a different topology of the active site and a marked divergence between the model and each individual template. The advantage of our multiple-template approach resides essentially in the availability of a final template that can be used to rebuild various mammalian cytochromes P450. Up to now there is no available crystal structure or structural model of human CYP3A5, CYP 3A7, CYP3A43 or other mammalian CYP3A.

More recently, two new bacterial P450 crystal structures emerged in the literature (Table 1): CYP51 (PDB code 1e9x), from *Mycobacterium tuberculosis*, that catalyzes the oxidative removal of 14α-methyl group from sterol precursors in sterol biosynthesis in yeast and fungi (ergosterol), plants (phytosterol) and mammals (cholesterol), for its potential in the design of antifungal agents (Podust et al. 2001). And CYP119 (PDB code 1f4t), from the thermophilic archaeon *Sulfolobus solfataricus*, the first P450 identified in *Archaea*, for its interest in

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understanding the enhanced thermal stability of the structure, especially in the region of the active site (Yano et al. 2000). Those two structures have been shown to exhibit the typical bacterial P450 fold, with some exceptions in the topology. They have not been included as structural templates in the modeling steps of the CYP3A4 model described in example 1. The names of newly discovered P450s follow the now accepted nomenclature of David R. Nelson (Nelson 1999).

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The protein databank (Brookhaven Protein Databank, http://www.rcsb.org/pdb/) currently indicates that there are 76 separate crystal structures available for the eight crystallized P450s, plus 7 crystal structures on hold (Sept 1st, 2002), the majority of which containing either bound substrates or inhibitors. Table 1 provides the relevant information about the structural templates used for human CYP3A model rebuilding. The idea behind homology modeling is that proteins belonging to the same functional class and showing a strong sequence identity, adopt a similar fold (review in (Hilbert et al. 1993)). Known analogous structures are then used to generate a template or parent structure for the unknown protein to be modeled. The reliability of the various methods employed depend mostly on the number of experimental 3D structures that can be aligned. Knowing that for pairs of distantly related proteins (with residue identity of about 20%) the regions having the same fold will represent less than half of each molecule, the regions where the folds differ will predominate, and the divergence of sequence must be compensated by a higher number of homologous proteins to align (Chothia and Lesk 1986). Below 50% of sequence identity, the deviation in structurally not conserved regions becomes significant, and loop regions are difficult to predict. It is generally accepted that below 20% of sequence identity, the prediction turns out to be hazardous, and fold assignment methods are best replaced by ab initio methods, that ideally attempt to predict the native structure only from the primary sequence of the protein to be modeled. But produced models so far had the correct fold for only a few small protein domains (Sanchez et al. 2000).

The strategy of model rebuilding in the P450 family is strongly driven by the low degree of homology between bacterial and mammal cytochrome P450s (Table 2).

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808	Swiss-Prot	CP37_	CP34_	CP51_	CPXW_ CPC5_	_	CPXA_	CPXL			NOR
epoo	entry name	HUMAN	HUMAN MYCTU		SULSO	RABIT	PSEPU	PSESP	BACME	SACER	FUSOX
n.s.	CP37_HUMAN		製造								
n.s.	CP34_HUMAN	88.4 % 501 aa									
1E9X	CP51_MYCTU (CYP51)	27.7 % 26.9 % 372 aa 405 aa	26.9 % 405 aa								
1F4T	CPXW_SULSO (CYP119)	24.5 % 330 aa	25.4 % 410 aa	25.7 % 385 aa							
1DT6	CPC5_RABIT (CYP2C5)	27.9 % 481 aa	27.9 % 28.4 % 481 aa 497 aa	23.4 % 427 aa	23.5 % 344 aa			·			
3CPP	CPXA_PSEPU (P450 cam)	23.3 % 335 aa	21.3 % 399 aa	21.9 % 407 aa	23.3 % 21.3 % 21.9 % 26.6 % 24.2 % 335 aa 399 aa 407 aa 387 aa 480 aa	24.2 % 480 aa					
ICPT	CPXL_PSESP (P450 terp)	24.8 % 452 aa	24.4 % 356 aa	27.8 % 446 aa	29.3 % 409 aa	24.4 % 451 aa	27.4 % 398 aa		THE CLUB AND A		
HPD-A	2HPD-A CPXB_BACME (P450 BM3)	31.8 % 409 aa	29.9 % 445 aa	27.1 % 443 aa	31.8 % 29.9 % 27.1 % 24.5 % 22.7 % 23.1 % 409 aa 445 aa 443 aa 396 aa 480 aa 485 aa	22.7 % 480 aa	23.1 % 485 aa	24.0 % 363 aa		The state of the s	
10XA	CPXJ_SACER (P450 eryF)	25.5 % 415 aa	26.0 % 334 aa	27.7 % 423 aa	25.5 % 26.0 % 27.7 % 30.8 % 24.4 % 24.0 % 28.6 % 415 aa 334 aa 423 aa 396 aa 443 aa 391 aa 420 aa	24.4 % 443 aa	24.0 % 391 aa	28.6 % 420 aa	22.6 % 389 aa		A-SHICEN MA
IROM	NOR_FUSOX (P450 nor)	23.7 % 354 aa	23.7% 22.9% 23.1% 354 aa 415 aa 442 aa	23.1 % 442 aa	23.7% 22.9% 23.1% 27.7% 354 aa 415 aa 442 aa 379 aa	27.7 % 21.4 % 379 aa 351 aa	29.0 % 379 aa	29.0 % 31.5 % 379 aa 409 aa	21.4 % 29.0 % 31.5 % 23.0 % 351 aa 379 aa 409 aa 265 aa	32.7 % 395 aa	

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Table 2: Sequence identities between the various crystallized cytochrome P450s and human CYP3A4 and CYP3A7 using BLOSUM 62 matrix (source LALIGN, http://www.infobiogen.fr/services/analyseq/cgi-bin/lfastap_in.pl, algorithm of

- Huang and Miller LALIGN that finds the best local alignments between two sequences, version 2.1u03 April 2000, published in *Adv. Appl. Math.* 1991, 12: 373-381). The P450 BM3 structure, Swissprot code name CPXB_BACME, corresponds to the structure of a fusion protein of P450 and a reductase domain, so that it displays twice the number of residues.
- Our global scheme, which steps are described hereafter, is founded on a combination of methods developed in the literature for different purposes in protein structure determination studies. The principle of the primary steps, until the generation of a correct alignment of P450 primary sequences, is described in Jean et al. 1997. The last steps are summarized in Loiseau 2002.
- Therefore, in a first object, the invention relates to a method for designing a 3-dimentional (3-D) model of a protein, the 3-D representation of at least three family members has already been experimentally obtained, [said 3-D representation presenting similarities], comprising the steps of:
- a. identification of common structural blocks (CSBs) among said members of said
 family,
 - **b.** alignment of the amino-acids primary sequence of said family members according to said structural similarities, represented by said CSBs, in order to obtain a first alignment,
 - c. alignment of said protein as compared on said first alignment, in order to obtain a second alignment, wherein:
 - i. alignment of said protein is performed in order to optimize the amino-acids alignment between said protein and said first alignment, when one or more consensus amino-acid exists in said aligned CSBs in said first alignment, and in the amino-acid sequence of said protein, said consensus amino-acids are anchors of said second alignment,

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ii. no insertion or deletion of amino-acids can be performed in the aligned CSBs, wherein insertion or deletions are possible in out-of-block regions, if better to align the primary amino-acids sequences,

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- d. definition of the 3-D structure of CSBs of said protein, according to the 3-D structure of the CSBs of said family members,
- e. definition of the global constraints (distance and angular constraints) derived from the comparisons of the structural templates in CSBs, and definition of the local
 constraints (distance and angular constraints) for the atoms of residues that are not structurally determined after step d. (that are not in the CSBs),
 - f. selection of rotamers,

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- g. determination of a family of 3-D model structures of said protein, taking into account said 3-D structure of CSBs obtained in step d., said global and local constraints defined in step e., and said rotamers defined in step f.,
- h. optimization of said family of 3-D models obtained in step g., by
- i discarding structures that present topological defects, and
- ii recalculating 3-D structures by taking electrostatic forces into account,

and performing the method again from step c. downward, with modifications in the alignment between the primary sequence of said protein and said first alignment, when the obtained model structures do not satisfactorily account for known mutations having biological effects.

In the present invention, the term "backbone atoms" refers to the C, N, C α , and O atoms of a protein that are common to all amino acid building blocks or involved in the peptide linkage. When the protein structure is described as a trajectory in internal coordinates such as α , τ angles, or is a low-resolution crystallographic structure, backbone atoms stand only for C α atoms of each residue.

In the present invention, the term "similarities" is used in the search for structural fragments conserved between the template proteins, that is fragments that have similar local trajectories in the backbone internal coordinate space. Two protein fragments have "similar" local trajectories when they are matched according to two adjustable parameters, the mesh and the margin (Jean et al. 1997).

In the present invention, the term "common structural blocks (CSB)" define the protein fragments of equal length that are found similar between all the template proteins in the internal coordinate representation.

In the present invention, the term "first alignment" refers to the alignment imposed by the CSBs, that is the structural alignment between template proteins defined by CSBs sequences. This alignment is totally independent on the primary sequence of the template proteins.

In the present invention, the term "out-of-block regions" designates all other protein fragments located out of and between the CSBs, *i.e.* that are not structurally conserved in the internal coordinate space. There is no information of sequence alignment for these regions (see in Figure 1 regions that are not colored), since they are not relevant for structural conservation. Out-of-block regions are passively reconstructed with the rest of the structure during the calculation steps.

In the present invention, the term "global constraints" refers to geometric constraints that are assigned to atoms of residues from CSBs, and that can be derived by computing all distance or angle information available within CSBs or between CSB.

In the present invention, the term "local constraints" refers to loose structural constraints that are assigned to residues of out-of-block regions, in order to restrict their backbone conformation to allowed regions of the Ramachandran diagram.

In the present invention, the term "rotamers" defines the low energy side-chain conformations of residues. The use of a library of rotamers allows determining or modeling a structure with the most likely side-chain conformations, saving time and producing a structure that is more likely to be correct.

20 For identification of CSBs between all selected 3D structures:

CSBs define the common local folds found similar in the template proteins, and are used as building blocks to set up the fold of the model (results in Loiseau 2002). The non conserved regions, that can be parts of secondary structures or non-structured regions as loops, will be rebuilt with no initial structural information.

For multiple alignment of crystalline P450s, on the basis of CSBs determination:

Once the structurally conserved elements are identified, a first structural alignment between the template proteins is derived. The following step involves the localization of these elements in the target sequence. Sequence pairwise comparisons between selected crystal structures and CYP3A (Table 2) show low sequence identity, so that online tools of multiple alignment such as CLUSTALW or PHD (Heidelberg) fail to produce an clear-cut alignment. Instead, local alignment tools, such as that described in Jean et al. 1997, were used to match the CSB profile to the target sequence, where a matrix is slid along the sequence and a

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score of similarity (based on a standard matrix such as BLOSUM62) is calculated for each position. Online tools of multiple alignment such as CLUSTALW 1.8 can be further used for assessment of accuracy.

The target sequence of human cytochrome P450 3A is thus aligned against the multiple alignment obtained from the CSBs. This produces the key sequence alignment which allows the generation of the template structure used for the rebuilding of the various CYP3A models. Following steps involve:

- 1) Generation of distance and dihedral angles constraints.
- 2) Selection of rotamers for side chains in CSBs.
- 3) Calculation of a set of structures using DYANA software. Loops are rebuilt between CSBs.
 - 4) Structure optimization under XPLOR software (Brünger 1992).

In a preferred embodiment, said 3-D representation of family members has been obtained by crystallography or NMR.

The alignment of said common structural blocks in steps **b.** and **c.** can be performed by use of the GOK software as described in Jean et al., 1997.

In addition, step d. is preferably performed according to the following rules:

- i. at a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the target residue,
- ii. When residues differ, only the coordinates of the backbone atoms are assigned $(C\alpha)$, and sometimes $C\beta$ or $C\gamma$ when they exist.

The definition of rebuilding global constraints in step e. is performed by using all available geometrical information intra- and inter-CSB (distances and angles), issued from the comparisons of the structural templates, each geometric constraint being defined as an interval. On another hand, the definition of local constraints for out-of-blocks residues is performed by analysis of the allowed regions in Ramachandran diagram.

Furthermore, distances and angles defining global constraints are preferably selected in step e. by the following rules:

- i. all distances for which the lower boundary is less than 8 Å,
- ii. all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs

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iii.all the distances involving atoms of any active group such as an heme group, to fix as much as possible the neighborhood of said active group, such as an iron atom.

The distance of 8 Å is chosen in order to reduce drastically the total number of constraints to take into account in the computation, and to allow to excessively constrain the model.

Angular constraints are preferably selected in step e. by the following rule:

i. dihedral angles ϕ and ψ of all residues located in CSBs are defined as constraints, given by the average values of corresponding ϕ , ψ angles in said family members +/- the calculated standard deviation.

To practice the method of the invention, rotamers in step f. can be selected from the couples according to the tables of Dunbrack and Karplus and step g. can be performed with the DYANA software, as described in Güntert et al, 1997.

In addition, the optimization in step h. comprises the use of the X-Plor software, as described in A. T. Brünger, X-PLOR, version 3.1.

The method according to the invention is particularly applicable to a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A]

In a preferred embodiment, said mammal cytochrome P450 3A is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29

(SEO ID N°17) and CYP3A13 (SEQ ID N°18). 20

In another preferred embodiment, said human cytochrome P450 subfamily 3A is selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13).

The method is applicable as well to human cytochrome of the subfamily P450 3A4, wherein said family members that are used for performing said first alignment for designing a 3-D model of CYP3A4 are chosen from Nor (SEQ ID N° 1), Ery F (SEQ ID N° 2), terp (SEQ ID N° 3), Cam (SEQ ID N° 4), BM3 (SEQ ID N° 5) and 2C5 (SEQ ID N° 6).

The method is applicable as well to human cytochrome of the subfamily 3A7, wherein family members that are used for performing said first alignment for designing a 3-D model of CYP3A7 are chosen from Ery F (SEQ ID N° 2), BM3 (SEQ ID N° 5), CYP51 (SEQ ID N° 8) and 2C5 (SEQ ID N° 6).

The method is applicable as well to other mammalian cytochrome P450 3A isoforms.

In a second object, the invention is directed to 3-D structure model of a protein, obtained by the method as described above.

- In a preferred embodiment, the protein is a cytochrome P450 subfamily 3A comprising mammal and human cytochromes P450 3A

 In another preferred embodiment, the protein is selected from the group comprising CYP3A6 (SEQ ID N°14), CYP3A12 (SEQ ID N°16), CYP3A29 (SEQ ID N°17) and CYP3A13 (SEQ ID N°18).
- In still another preferred embodiment, the protein is a human cytochrome P450 subfamily 3A selected from the group comprising CYP3A4 (SEQ ID N°11), CYP3A7 (SEQ ID N°15), CYP3A5 (SEQ ID N°12) and CYP3A43 (SEQ ID N°13). In still another preferred embodiment, the protein is a human cytochrome P450 3A4 or 3A7.
- Regarding the rebuilt P450 3A4 model, the main residues involved in the recognition of the substrate are C97; R104; F101; F107; F247; F303 and C376.

 More specifically, C97 and C376 are found in positions compatible with the formation of a disufide bridge allowing limited or enhanced flexibility of corresponding protein domains, while R104 is involved in the capture of the substrate that is close to the entrance site, and allows to accompany it to the active site. F303 is involved in the recognition of the substrate in the active site. F107; F247 and F303 are involved in the recognition at the modulation site responsible for positive regulation. Role of F303 in the active site has already been suggested by studies of Domanski et al. 1998 in the SRS 4 region (mutants I300, F303, A304, and T308).

Features of this model comprise the 3-D atomic coordinates of **Table 3**. Table 3

In a preferred embodiment, the residues C97; R104; F101; F107; F247; F303 and C376 are involved in the CYP 3A4 for the recognition and uptake of the substrate at the entry site, and its binding into the active site having the 3-D atomic coordinates of Table 3.

Regarding the P450 3A7 model, features comprise the 3-D atomic coordinates of **Table 4**.

Table 4

In a preferred embodiment the residues Q79; F102; R105; R106; F108; F248; F304 and E374 are involved in the CYP 3A7 for the recognition and uptake of the substrate at the entry site, and its binding into the active having the 3-D atomic coordinates of Table 4.

In a third object, the invention contemplates a method for designing a protein, biological functions of which are altered, comprising:

- a) obtaining a 3-D model of said protein by the method as depicted above,
- b) analyzing said model of step a., and determining the amino-acids that are putatively involved in the biological functions of said protein,
 - c) changing said amino-acids by mutating the corresponding nucleotides on the nucleic acid sequence coding for said protein, in order to obtain a mutated protein having altered properties.

In the present invention, the term "altered properties" means that the generated protein is altered in its enzymatic properties, such as the substrate recognition, the movements associated to the entrance or the exit of the substrate, the multiple binding at the active site, the allosteric behaviour, the electron transfer, the coupling to the P450 reductase.

In another object, the invention relates to a computer-assisted method for performing restrained dynamics docking of a substrate on an enzyme, a 3-D structure of which is available, comprising the steps:

- j. determining a force field, and independently simulating the presence of said enzyme in said force field,
- k. minimizing the potential energy (Ep) linked to said force field of said 3-D structure, wherein the spatial position of some atoms of said enzyme is fixed, and wherein the other atoms are mobile, by allowing mobility of the mobile atoms, by i. simulating an increase in temperature (in order to give kinetic energy),
 - ii. and minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- 30 l. optionally repeating step k in order to obtain other Ep minima, wherein said Ep minima are such that the structure of the protein remains folded,
 - m. minimizing Ep in said force field of said 3-D structure, wherein all the atoms of the protein are mobile, by

- i. simulating an increase in temperature (in order to give kinetic energy), and
- ii. minimizing the potential energy by re-specifying the temperature as 0 Kelvin (K)
- n. simulating, at 0 K the presence of said substrate next to said enzyme,
- o. optionally generating a molecular dynamics simulation on said substrate and enzyme (simulating an increase in temperature, in order to allow mobility of the atoms)
 - **p.** generating some constraints to said substrate, in order to impose that it has interaction with said enzyme,
- q. generating a molecular dynamics simulation on said substrate and enzyme, with said constraints imposed in step p.,
 - r. optionally, generating a molecular dynamics simulation on said substrate and enzyme without said constraints of step p.

In the present invention, the term "restrained dynamics docking" means a procedure by which the docking of the substrate is simulated using molecular dynamics (MD) simulations under constraints that are specified by the user.

- In the present invention, the term "soft-restrained dynamics docking" refers to a restrained dynamics docking in which the substrate-protein distance constraints are loose, with force field parameters associated to the constraints as low as 1 or 2 Kcal/mol.
- In the present invention, the term "constraints" when applied to substrate docking refers to a distance imposed between atoms of the protein, generally from the active site (such as atoms of the heme group), and atoms of the substrate. These distance restraints are defined as intervals, where the distance range is large enough to allow the free movement of the substrate within the active site.
- In a preferred embodiment of this method for performing restrained dynamics docking, said fixed atoms in step **k**. are the backbone atoms N-Cα-CO in the first minimization step and only Cα in subsequent minimization steps.

In another preferred embodiment of this method, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

- 30 The force field in step j. comprises forces linked to:
 - a. the distance between atoms,
 - b. the angles of valence,
 - c. the dihedral angles,

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- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- g. hydrogen bonds.
- The constraints in step p. are attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.
- In the present invention, the term "final distance constraints", when applied to substrate docking, means distances imposed between atoms from the heme group (such as the iron atom), and atoms of the substrate. These distance contraints are defined as intervals, and are related to the final position of the substrate in the vicinity of the heme group before metabolization.
- Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.
 - This method is particularly suited for multispecific protein such as a cytochrome 36

 P450 subfamily 3A comprising mammal and human cytochromes.
 - The cytochrome can be cytochrome P450 3A4 or any of all other P450 from the 3A subfamily, and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.
- The substrate can be a small organic compound which size can range for example from MW 288 (testosterone) to MW 1203 (cyclosporine A).
 - In a preferred embodiment said substrate is testosterone.

molecular dynamics simulations.

In another object, the invention is aimed at a computer-assisted method for performing restrained dynamics docking of at least two substrates on an enzyme, a 3-D structure of which is available, consisting of performing the steps **j**, **k**, **l**, **m**, **n**, **o**, **p**, **q** and **r** depicted above with a first substrate and repeating said steps with a second substrate when the first substrate reaches an unconstrained state after

The first and second substrates can be the same molecule or different molecules.

The first and second substrates can display either allosteric or synergistic effect.

This method can be practiced with substrates that are inhibitors (competitive, uncompetitive, non competitive) or display an inhibitor-base mechanism. It can also

5 be practiced with an agonist and any molecule interfering with the biological function of the protein.

In preferred embodiments:

- the first and second substrates are the same molecule.
- the first and second substrates are different molecules.
- 10 the first and second substrates display an allosteric effect.
 - the first and second substrates display a synergistic effect.
 - at least one of the substrates is an inhibitor or display an inhibitor-based mechanism.
 - at least one of the substrates is an agonist.
- In another embodiment, this method also embraces a successive repeat of the steps j, k, l, m, n, o, p, q and r depicted above with a 3rd, 4th or 5th substrate, some of them being the same or different molecules.

In this method for performing restrained dynamics docking, said fixed atoms in step \mathbf{k} . are the backbone atoms N-C α -CO in the first minimization step and only C α in subsequent minimization steps.

In addition, kinetic energy is simulated by temperature increase to about 100 K for about 5-20 ns.

The force field in step j. comprises preferably forces linked to

- a. the distance between atoms,
- b. the angles of valence,

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- c. the dihedral angles,
- d. the deformation with regard to planar geometry,
- e. the electrostatic field,
- f. the Van der Waals forces,
- 30 g. hydrogen bonds.

The constraints in step **p**. are preferable attraction constraints to force said substrate in the active site, and wherein said constraints are not prejudiced to the exact spatial conformation of the substrate in the active site. These constraints are final distance

constraints between some atoms of said substrate and some atoms of amino-acids present in said active site.

Preferably, step o. is performed with a simulated temperature of between about 15 and 50 K, step q. is performed with a simulated temperature of between about 15 and 50 K, and step r. is performed with a simulated temperature of between about 200 and 350 K.

This method is particularly suited for multispecific protein such as a cytochrome P450. The cytochrome can be cytochrome P450 3A4, or any of all other P450 of the 3A subfamily and said structure can be the structure obtained by the method of the invention described above, in particular the model structures which atomic coordinates are listed in Tables 3 and 4 for CYP3A4 and CYP3A7.

In a preferred embodiment:

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- said cytochrome is cytochrome P450 3A4, and said structure is the structure obtained by the above-described method, in particular the above-described model structure,
- said first and second substrates are small organic compounds which size can range from MW 288 (testosterone) to MW 1203 (cyclosporine A),
- said substrate is testosterone.

The invention is also directed to the use of the method for designing a 3-D model of a protein and to the computer-assisted method for performing restrained dynamics docking as mentioned above for screening, designing or identifying natural, unnatural substrates or substrate analogs, as well as inhibitors, activators or modulators of said enzyme.

Another object of the invention is the use of these methods for determining the effect of a first substrate on a second substrate, which can also be applied to pharmaceutical products.

The invention contemplates the use of these methods for determining the effect of a first bound testosterone molecule on the access of a second testosterone molecule as well as for determining the mutual effect of a testosterone molecule with alphanaphtoflavone (αNF) molecule.

The invention is also directed to:

- * The use of the above described computer-assisted methods for determining the oxidative modification of the substrate according to the proximity to the heme of a part of the substrate to give rise to metabolite.
- The oxidized or reduced molecule derived from a given substrate modified after positioning at the right distance to the heme is called metabolite.

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- * The use of the above described computer-assisted methods, for performing dynamic docking of the said metabolite, either in the absence or in the presence of the second substrate in the calculation.
- * The use of the above described computer-assisted methods for dynamic docking to compare the energy of the bound metabolite relatively to the energy of its parent substrate bound, in order to determine if the exit of the given metabolite from the enzyme is favored or not.
 - * The use of the above described computer-assisted methods for dynamic docking to study the different exit pathways that are accessible to the metabolite, either in the absence or in the presence of the second substrate in the calculation.

The distance and angular constraints derived from CSBs common to the crystallized cytochromes P450 used as structural templates, are applied to conserved atoms of CSBs of the target protein. The DYANA software (Güntert et al. 1997) allows to rebuild directly the whole structure of the target protein on the basis of its primary sequence, by taking into account these geometric constraints. Out-of-blocks residues are rebuilt *ab initio* by selecting the most favorable solutions in terms of minimal global potential energy. As examples, actual tables 3 and 4 display the atomic coordinates of structural models obtained by applying DYANA calculation to target protein sequences CYP3A4 and CYP3A7 respectively.

TABLE 3	. D		+ h o	coord	inatee	of t	ha C	V D Z A	4 mo	del						
HEADER	CYP		the	COOLG	Inaces	01 (ne c	11 50	7 11.0							
TITLE	MOD	EL OF	HUMA	N CYT	OCHROM	E P45	0 CY	P3A4								
AUTHOR	N.	LOISE	All.F.	ANDRE	.C.MIN	OLETT	'I.M.	DELA	FORG	E			CT !!	ave		
SEQRES	1	452	SER	TYR H	IS LYS	GLY	PHE	CYS	MET	PHE .	ASP	MET	760	CIS		
SEQRES	2	452	HIS	LYS L	YS TYR RO VAL	GLY	LYS	VAL	TKP	ACD.	DDO DDO	D C D	MET	TLE		
SEQRES	3	452	GLN	GLN P	RO VAL	LEU	ALA	LLE	CVE	TVD	SEB	VAT.	PHE	THR		
SEQRES	4	452	LYS	THE V	RG PRO	AND	CLY	DBU GTO	VAI.	GLY	PHE	MET	LYS	SER		
SEQRES	5 6	452 452	ASN	TLE S	ER ILE	AT.A	GLU	ASP	GLU	GLU	TRP	LYS	ARG	LEU		
SEQRES SEQRES	7	452	ARG	SER L	EU LEU	SER	PRO	THR	PHE	THR	SER	GLY	LYS	LEU		
SEQRES	8	452	LYS	GLU M	ET VAL	PRO	ILE	ILE	ALA	GLN	TYR	GLY	ASP	VAL		
SEQRES	9	452	LEU	VAI. A	RG ASN	LEU	ARG	ARG	GLU	ALA	GLU	THR	GLY	LYS		
SEQRES	10	452	PRO	VAL 1	HR LEU	LYS	ASP	VAL	PHE	GLY	ALA	TYR	SER	MET		
SEQRES	11	452	ASP	VAL I	LE THE	SER	THR	SER	PHE	GLY	VAL	CLU	JEN	THR		
SEQRES	12	452	SER	LEU A	LEU LEU	ARC	OPE	ASP	PHE	LEU	ASP	PRO	PHE	PHE		
SEQRES	13	452 452	LYS	PIO I	LE THE	VAL.	PHE	PRO	PHE	LEU	ILE	PRO	ILE	LEU		
SEQRES SEQRES	14 15	452	CUI	VAI. I	EU ASN	ILE	CYS	VAL	PHE	PRO	ARG	GLU	VAL	THR		
SEQRES	16	452	ASN	PHE I	EU ARC	LYS	SER	VAL	LYS	ARG	MET	LYS	GLU	SER		
SEQRES	17	452	ARG	LEU (LU ASI	THR	GLN	LYS	HIS	ARG	VAL	ASP	PHE	LEU		
SEQRES	18	452	GLN	LEU N	MET ILE	ASP	SER	GLN	ASN	SER	LYS	GLU	THR	GLU		
SEQRES	19	452	SER	HIS I	LYS ALA	LEU	SER	ASP	LEU	GLU	LEU	VAL	ALA	GLN		
SEQRES	20	452	SER	ILE 1	LE PH	ILE	PHE	ALA	GLY	TYR	GLU	THE	THE	DER		
SEQRES	21	452	SER	VAL 1	LEU SEI VAL GLI	PHE	ILE	MET	CIM	CLU	CITI	TLE	ACD	A1.A		
SEQRES	22	452	PRO	ASP	PRO ASI	I TVS	DIS	PEO	PRO	THR	TYR	ASP	THR	VAL		
SEQRES	23 24	452 452	VAL	CIN I	MET GL	ים אי	LEU	ASP	MET	VAL	VAL	ASN	GLU	THR		
SEQRES SEQRES	25	452	LEU	ARG :	LEU PHI	E PRO	ILE	ALA	MET	ARG	LEU	GLU	ARG	VAL		
SEQRES	26	452	CYS	LYS	LYS AS	P VAI	. GLU	ILE	ASN	GLY	MET	PHE	ILE	PRO		
SEQRES	27	452	LYS	GLY '	TRP VA	LVAI	MET	ILE	PRC	SER	TYR	ALA	LEU	HIS		
SEQRES	28	452	ARG	ASP	PRO LY	STYF	TRP	THR	GLU	PRO	GLU	LYS	PHE	LEU		
SEQRES	29	452	PRO	GLU .	ARG PH	E SEF	LYS	LYS	ASN	LYS	ASP	ASN	175	ASP		
SEQRES	30	452	PRO	TYR	ILE TY GLY ME	R THE	. BRC) PME	LEU	DER MET	DSN	MET	LYS	LEU		
SEQRES	31 32	452 452	CYS	100	ILE AR	I AN	. LEU	GLN	ASN	PHE	SER	PHE	LYS	PRO		
SEQRES SEQRES	33	452	CYS	LYS	GLU TH	R GLI	ILE	: PRO	LEU	J LYS	LEU	SER	LEU	J GLY		
SEQRES	34	452	GLY	LEU	LEU GL	N PRO	GLU	LYS	PRO) VAL	VAL	LEU	LYS	S VAL		
SEQRES	35	452	GLU	SER	ARG AS	P GL	THF	VAL	SEF	R GLY	ALA					
HET	HEM	600														
HETNAM	HEM	HEM	E	_							2025	NI T NI E	ים דם:	OTRO	MIC	act D
HETSYN					RAMETH	AP-8	, 13-L)T A T K	111,-4	2,10-	PORE	LUTINE	SDIF:	NOF TO		
FORMUL	HEM 1	N C 3 4	SER	N4 O4 51	L E-T	9.99	9 -	.760) -	4.543	1.	.00	0.0	0		3A4
ATOM ATOM	2	CA	SER	51	1	0.71		.477		4.293		.00	0.0	0		3A4
ATOM	3	СВ	SER	51		9.94		731		4.939	1.	.00	0.0	0		3A4
ATOM	4	OG	SER	51		8.60	1 (3.876		4.493		.00	0.0			3A4
ATOM	5	С	SER	51		0.96		281		2.815		.00	0.0			3A4 3A4
MOTA	6	0	SER	51		0.27		0.855		1.969	•	.00 .00	0.0			3A4
ATOM	7	N	TYR	52		1.97 2.43		0.569 0.860		2.482 1.131		.00	0.0			3A4
ATOM	8 9	CA CB	TYR TYR	52 52		3.98		0.783		0.979		.00	0.0			3A4
ATOM ATOM	10	CG	TYR	52		4.45		0.57		1.430		.00	0.0			3A4
ATOM	11		TYR	52		4.14		1.73		0.69		.00	0.0			3A4
ATOM	12		TYR	52	1	5.21		0.70		2.61		.00	0.0			3A4
ATOM	13	CE1	TYR	52		4.57		2.99		1.13		.00	0.0			3A4 3A4
MOTA	14		TYR	52		5.65		1.95		3.05		.00	0.0			3A4
ATOM	15	CZ	TYR	52		5.33		3.10 4.37		2.31		.00	0.0			3A4
ATOM	16	ОН	TYR	52 52		l5.78 l1.97		2.24		0.75		.00	0.0			3A4
ATOM ATOM	17 18	С 0	TYR TYR	52 52		L2.17		3.20		1.49		.00	0.0			3A4
ATOM	19	N	HIS	53		11.32		2.35		0.42		.00	0.0			3A4
ATOM	20	CA	HIS	53		10.74		3.56		0.95		.00	0.0			3A4
ATOM	21		HIS	53		7.85		1.85		1.03		.00	0.0			3A4
MOTA	22	CG	HIS	53		8.48		2.63		0.09		.00	0.0			3A4 3A4
ATOM	23	CB	HIS	53		9.32		3.86		0.38 se o-		.00	0.0			3A4
ATOM	24		HIS	53 53		7.43 8.23		0.92		-0.93 -1.10		.00	0.0			3A4
MOTA MOTA	25 26		HIS HIS	53 53		7.24		0.84	-	0.36		.00	0.0			3A4
ATOM	26 27	CEI	HIS	53		10.7		3.38		2.44		1.00	0.	00		3A4
ATOM	28	ŏ	HIS	53		9.7		3.18	13	3.08		1.00	0.			3A4
ATOM	29	N	LYS	54		11.9	73	3.46	51	3.04	3 1	1.00	0.	υŪ		3A4

ATOM	30	CA	LYS	54	12.265	3.262	4.451	1.00	0.00	3A4
ATOM	31	СB	LYS	54	13.401	2.217	4.659	1.00	0.00	3A4
MOTA	32	CG	LYS	54	13.053	0.819	4.120	1.00	0.00	3A4
ATOM	33	CD	LYS	54	14.220	-0.183	4.148	1.00	0.00	3A4 3A4
MOTA	34	CE	LYS	54	14.793	-0.500 -1.087	5.540 6.431	1.00	0.00	3A4 3A4
ATOM ATOM	35 36	NZ C	LYS LYS	54 54	13.763 12.660	4.603	5.025	1.00	0.00	3A4
ATOM	37	Ö	LYS	54	13.829	4.851	5.317	1.00	0.00	3A4
ATOM	38	N	GLY	55	11.656	5.510	5.181	1.00	0.00	3A4
ATOM	39	CA	GLY	55	11.819	6.901	5.560	1.00	0.00	3A4
ATOM	40	С	GLY	55	11.464	7.113	7.003	1.00	0.00	3A4
ATOM	41	0	GLY	55	10.305	7.002	7.400	1.00	0.00	3A4
ATOM	42	N	PHE	56	12.502	7.439	7.817	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	43 44	CA CB	PHE	56 56	12.451 13.646	7.714 7.051	9.250 10.010	1.00	0.00	3A4
ATOM	45	CG	PHE	56	13.966	5.681	9.448	1.00	0.00	3A4
ATOM	46		PHE	56	15.250	5.415	8.926	1.00	0.00	3A4
ATOM	47		PHE	56	12.987	4.669	9.370	1.00	0.00	3A4
ATOM	48	CEl	PHE	56	15.543	4.185	8.320	1.00	0.00	3A4
ATOM	49		PHE	56	13.271	3.445	8.747	1.00	0.00	3A4
ATOM	50	cz	PHE	56	14.550	3.205	8.224	1.00	0.00 0.00	3A4 3A4
ATOM	51	C	PHE	56 56	12.446 11.957	9.211 9.670	9.542 10.570	1.00	0.00	3A4
ATOM ATOM	52 53	O N	PHE	50 57	12.971	10.054	8.624	1.00	0.00	3A4
ATOM	54	CA	CYS	57	13.048	11.500	8.782	1.00	0.00	3A4
ATOM	55	СВ	CYS	57	13.902	12.161	7.665	1.00	0.00	3A4
ATOM	56	SG	CYS	57	15.312	11.121	7.176	1.00	0.00	3A4
ATOM	57	С	CYS	57	11.705	12.171	8.760	1.00	0.00	3A4
ATOM	58	0	CYS	57	11.446	13.160	9.434	1.00	0.00 0.00	3A4 3A4
ATOM	59	N	MET	58 58	10.778 9.402	11.585 12.000	7.975 7.870	1.00	0.00	3A4
ATOM ATOM	60 61	CA CB	MET MET	58	8.715	11.289	6.694	1.00	0.00	3A4
MOTA	62	CG	MET	58	9.360	11.641	5.343	1.00	0.00	3A4
ATOM	63	SD	MET	58	8.469	11.004	3.887	1.00	0.00	3A4
ATOM	64	CE	MET	58	8.922	9.256	4.080	1.00	0.00	3A4
MOTA	65	С	MET	58	8.612	11.706	9.122	1.00	0.00	3A4
ATOM	66	0	MET	58	7.740	12.480	9.487	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	67 68	N CA	PHE	59 59	8.963 8.394	10.612 10.230	9.844 11.122	1.00	0.00	3A4
ATOM	69	CB	PHE	59	8.732	8.752	11.449	1.00	0.00	3A4
ATOM	70	CG	PHE	59	7.865	8.152	12.538	1.00	0.00	3A4
ATOM	71	CD1	PHE	59	6.477	8.002	12.350	1.00	0.00	3A4
MOTA	72		PHE	59	8.430	7.747	13.764	1.00	0.00	3A4
ATOM	73		PHE	59	5.671	7.462	13.364 14.780	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	74 75	CE2	PHE	59 59	7.627 6.247	7.208 7.065	14.579	1.00	0.00	3A4
ATOM	76	c	PHE	59	8.881	11.119	12.255	1.00	0.00	3A4
ATOM	77	ō	PHE	59	8.110	11.479	13.139	1.00	0.00	3A4
ATOM	78	N	ASP	60	10.162	11.568		1.00	0.00	3A4
ATOM	79	CA	ASP	60	10.690	12.515	13.200	1.00	0.00	3A4
ATOM	80	CB	ASP	60	12.225	12.651 11.313	13.131	1.00	0.00	3A4 3A4
ATOM ATOM	81 82	CG OD1	ASP ASP	60 60	12.906 12.613	10.736	14.532	1.00	0.00	3A4
ATOM	83		ASP	60	13.743	10.859	12.624	1.00	0.00	3A4
ATOM	84	C	ASP	60	10.102	13.900	13.031	1.00	0.00	3A4
ATOM	85	٥	ASP	60	9.841	14.603	14.000	1.00	0.00	3A4
MOTA	86	N	MET	61	9.809	14.318	11.780	1.00	0.00	3A4
MOTA	87	CA	MET	61	9.130	15.564	11.481	1.00	0.00	3A4 3A4
ATOM	88	CB CG	MET	61 61	9.224 10.590	15.881 16.349	9.987 9.497	1.00	0.00	3A4
ATOM ATOM	89 90	SD	MET MET	61	10.659	16.502	7.686	1.00	0.00	3A4
ATOM	91	CE	MET	61	12.223	17.411	7.689	1.00	0.00	3A4
ATOM	92	c	MET	61	7.653	15.548	11.870	1.00	0.00	3A4
ATOM	93	0	MET	61	7.073	16.551	12.274	1.00	0.00	3A4
ATOM	94	N	GLU	62	7.012	14.358	11.819	1.00	0.00	3A4
ATOM	95	CA	GLU	62	5.653	14.159	12.272	1.00	0.00	3A4 3A4
ATOM	96 97	CB CG	GLU GLU	62 62	5.077 4.640	12.770 12.657	11.933 10.462	1.00	0.00	3A4 3A4
ATOM ATOM	98	CD	GLU	62 62	4.351	11.190	10.120	1.00		3A4
ATOM	99		GLU	62	3.429	10.603	10.748	1.00		3A4
ATOM	100		GLU	62	5.048	10.637	9.227	1.00		3A4
MOTA	101	С	GLU	62	5.522	14.338	13.751	1.00	0.00	3A4

ATOM	102	0	GLU	62	4.508	14.819	14.225	1.00	0.00	3A4
ATOM	103	N	CYS	63	6.605	14.104	14.522	1.00	0.00	3A4
MOTA	104	CA	CYS	63	6.664	14.441	15.921	1.00	0.00	3A4 3A4
MOTA	105	CB	CYS	63	7.902	13.805	16.588	1.00	0.00	3A4
MOTA	106	SG	CYS	63	7.977 6.526	11.995 15.952	16.382 16.211	1.00	0.00	3A4
MOTA	107	C O	CYS CYS	63 63	6.277	16.322	17.335	1.00	0.00	3A4
ATOM ATOM	108 109	N	HIS	64	6.436	16.853	15.182	1.00	0.00	3A4
MOTA	110	CA	HIS	64	5.487	17.970	15.236	1.00	0.00	3A4
ATOM	111		HIS	64	4.140	20.440	16.744	1.00	0.00	3A4
ATOM	112	CG	HIS	64	5.232	20.460	15.904	1.00	0.00	3A4
ATOM	113	CB	HIS	64	6.151	19.284	15.666	1.00	0.00	3A4
ATOM	114		HIS	64	4.280	22.506	15.939	1.00	0.00	3A4
MOTA	115		HIS	64	5.301	21.731	15.420	1.00	0.00	3A4 3A4
ATOM	116		HIS	64	3.608	21.687 18.138	16.726 13.901	1.00	0.00	3A4
ATOM	117	С	HIS	64 64	4.780 3.812	17.438	13.610	1.00	0.00	3A4
ATOM ATOM	118 119	O N	HIS LYS	65	5.240	19.107	13.073	1.00	0.00	3A4
ATOM	120	CA	LYS	65	4.699	19.426	11.766	1.00	0.00	3A4
ATOM	121	СВ	LYS	65	3.264	20.052	11.761	1.00	0.00	3A4
ATOM	122	CG	LYS	65	2.994	21.171	12.783	1.00	0.00	3A4
ATOM	123	CD	LYS	65	1.557	21.704	12.722	1.00	0.00	3A4
ATOM	124	CE	LYS	65	1.220	22.723	13.820	1.00	0.00	3A4
MOTA	125	NZ	LYS	65	2.052	23.944	13.700	1.00	0.00	3A4 3A4
ATOM	126	C	LYS	65	5.705	20.365	11.146 9.944	1.00	0.00 0.00	3A4
ATOM	127	0	LYS	65 66	5.958 6.332	20.315 21.227	12.000	1.00	0.00	3A4
ATOM ATOM	128 129	N CA	LYS LYS	66	7.517	22.020	11.730	1.00	0.00	3A4
ATOM	130	СВ	LYS	66	7.373	23.548	12.037	1.00	0.00	3A4
ATOM	131	CG	LYS	66	6.519	24.352	11.039	1.00	0.00	3A4
MOTA	132	CD	LYS	66	5.001	24.175	11.175	1.00	0.00	3A4
ATOM	133	CE	LYS	66	4.191	25.119	10.278	1.00	0.00	3A4
MOTA	134	NZ	LYS	66	2.736	24.881	10.442	1.00	0.00	3A4 3A4
ATOM	135	С	LYS	66	8.551	21.370	12.620 12.253	1.00	0.00 0.00	3A4
ATOM	136	0	LY5	66 67	9.100 8.772	20.332 21.934		1.00	0.00	3A4
ATOM	137 138	N CA	TYR TYR	67 67	9.441	21.263	14.936	1.00	0.00	3A4
ATOM ATOM	139	CB	TYR	67	11.005	21.348	14.926	1.00	0.00	3A4
ATOM .	140	CG	TYR	67	11.555	20.265	14.028	1.00	0.00	3A4
MOTA	141		TYR	67	11.325	18.909	14.336	1.00	0.00	3A4
ATOM	142	CD2	TYR	67	12.250	20.569	12.847	1.00	0.00	3A4
MOTA	143		TYR	67	11.798	17.884	13.506	1.00	0.00	3A4 3A4
ATOM	144	CE2		67	12.720	19.550	12.006	1.00	0.00	3A4
ATOM	145	CZ OH	TYR	67 67	12.507 13.010	18.207 17.184	12.342 11.509	1.00	0.00	3A4
ATOM ATOM	146 147	C	TYR TYR	67	8.880	21.880	16.194	1.00	0.00	3A4
ATOM	148	ŏ	TYR	67	8.905	23.092	16.404	1.00	0.00	3A4
ATOM	149	N	GLY	68	8.343	20.969	17.043	1.00	0.00	3A4
MOTA	150	CA	GLY	68	7.620	21.161	18.278	1.00	0.00	. 3A4
MOTA	151	C	GLY	68	8.251	20.139	19.164	1.00	0.00	3A4
ATOM	152	0	GLY	68	8.314	18.954	18.839	1.00	0.00	3A4 3A4
ATOM	153	N	LYS	69	8.864 10.301	20.642	20.260	1.00	0.00	3A4
ATOM	154	CA CB	LYS LYS	69 69	10.301	20.592 21.997	20.404		0.00	3A4
ATOM ATOM	155 156	CG	LYS	69	10.733	23.112	19.844		0.00	3A4
ATOM	157	CD	LYS	69	10.770	24.527	20.225		0.00	3A4
ATOM	158	CE	LYS	69	9.876	25.161	21.300	1.00	0.00	3A4
ATOM	159	NZ	LYS	69	10.236	26.582	21.514		0.00	3A4
MOTA	160	С	LYS	69	10.811	19.541	21.360			3A4
MOTA	161	0	LYS	69	11.914	19.033	21.177		0.00	3A4 3A4
ATOM	162	N	VAL	70	10.033	19.200	22.410			3A4
ATOM	163	CA	VAL	70 70	10.427 10.984	18.227 18.837	23.408 24.696			3A4
ATOM	164 165	CB	VAL 1 VAL	70 70	12.504	18.835	24.571			3A4
ATOM ATOM	166		VAL VAL	70 70	10.344	20.206				3A4
ATOM	167	c c	VAL	70	9.212					3A4
ATOM	168	ŏ	VAL	70	8.176			1.00		3A4
ATOM	169	N	TRP	71	9.337					3A4
MOTA	170	CA	TRP	71	8.255					3A4
ATOM	171	СВ	TRP	71	7.614					3A4 3A4
ATOM	172	CG	TRP	71	6.390					3A4 3A4
MOTA	173	CD	2 TRP	71	5.135	14.145	22.880	, 1.00	, 0.00	JAN

ATOM	174	CD1	TRP	71	6.251	12.660	21.615	1.00	0.00	3A4
ATOM	175	NE1		71	4.996	12.146	21.846	1.00	0.00	3A4
MOTA	176	CE2	TRP	71	4.292	13.040	22.624	1.00	0.00	3A4
MOTA	177	CE3	TRP	71	4.695	15.227	23.643	1.00	0.00	3A4
MOTA	178	CZ2		71	2.995	12.995	23.131	1.00	0.00	3A4
ATOM	179	CZ3		71	3.388	15.180	24.153	1.00	0.00	3A4
MOTA	180	CH2		71	2.551	14.080	23.902	1.00	0.00	3A4 3A4
ATOM	181	C	TRP	71	8.828	13.911	24.261 24.059	1.00	0.00	3A4
ATOM	182	0	TRP	71 72	9.989 7.987	13.584 13.188	25.027	1.00	0.00	3A4
ATOM ATOM	183 184	N CA	GLY	72	8.345	11.936	25.647	1.00	0.00	3A4
ATOM	185	C	GLY	72	7.812	10.809	24.804	1.00	0.00	3A4
ATOM	186	ŏ	GLY	72	6.679	10.850	24.336	1.00	0.00	3A4
ATOM	187	N	PHE	73	8.645	9.773	24.586	1.00	0.00	3A4
ATOM	188	CA	PHE	73	8.334	8.591	23.820	1.00	0.00	3A4
ATOM	189	CB	PHE	73	9.278	8.443	22.586	1.00	0.00	3A4
MOTA	190	CG	PHE	73	8.893	7.320	21.647	1.00	0.00	3A4
MOTA	191		PHE	73	9.691	6.162	21.549	1.00	0.00	3A4
ATOM	192		PHE	73	7.717	7.398	20.877	1.00	0.00	3A4 3A4
ATOM	193		PHE	73	9.320	5.105	20.707 20.030	1.00 1.00	0.00 0.00	3A4
ATOM	194		PHE	73 73	7.344 8.146	6.343 5.196	19.947	1.00	0.00	3A4
ATOM ATOM	195 196	CZ C	PHE	73 73	8.515	7.451	24.788	1.00	0.00	3A4
ATOM	197	ö	PHE	73	9.257	7.543	25.757	1.00	0.00	3A4
ATOM	198	N	TYR	74	7.826	6.328	24.540	1.00	0.00	3A4
ATOM	199	CA	TYR	74	7.884	5.174	25.397	1.00	0.00	3A4
ATOM	200	СВ	TYR	74	6.631	5.032	26.304	1.00	0.00	3A4
MOTA	201	CG	TYR	74	5.298	5.291	25.625	1.00	0.00	3A4
MOTA	202		TYR	74	4.515	4.223	25.146	1.00	0.00	3A4
MOTA	203		TYR	74	4.797	6.603	25.491	1.00	0.00	3A4
ATOM	204		TYR	74	3.279	4.456	24.524	1.00	0.00	3A4 3A4
ATOM	205		TYR	74 74	3.564 2.804	6.844 5.769	24.870 24.384	1.00	0.00	3A4
ATOM ATOM	206 207	CZ OH	TYR TYR	74	1.560	6.006	23.757	1.00	0.00	3A4
ATOM	208	C	TYR	74	8.100	4.007	24.486	1.00	0.00	3A4
ATOM	209	ŏ	TYR	74	7.256	3.682	23.658	1.00	0.00	. 3A4
ATOM	210	N	ASP	75	9.272	3.357	24.603	1.00	0.00	3A4
ATOM	211	CA	ASP	75	9.664	2.238	23.778	1.00	0.00	3A4
ATOM	212	СВ	ASP	75	11.110	2.479	23.220	1.00	0.00	3A4
ATOM	213	CG	ASP	75	11.483	1.556	22.044	1.00	0.00	3A4
MOTA	214		ASP	75	10.755	1.577	21.015	1.00	0.00	3A4
MOTA	215		ASP	75 75	12.500	0.822	22.166 24.657	1.00	0.00	3A4 3A4
ATOM	216 217	С 0	ASP ASP	75 75	9.580 9.275	1.007	25.845	1.00	0.00	3A4
MOTA MOTA	218	N	GLY	75 76	9.925	-0.191	24.123	1.00	0.00	3A4
ATOM	219	CA	GLY	76	10.101	-1.403	24.908	1.00	0.00	3A4
ATOM	220	C	GLY	76	11.420	-1.335	25.643	1.00	0.00	3A4
ATOM	221	Ó	GLY	76	12.463	-1.562	25.039	1.00	0.00	3A4
MQTA	222	N	GLN	77	11.349	-0.928	26.946	1.00	0.00	3A4
ATOM	223	CA	GLN	77	12.393	-0.521	27.882	1.00	0.00	3A4
ATOM	224	СВ	GLN	77	13.760	-1.300	27.835	1.00	0.00	3A4
ATOM	225	CG	GLN	77	14.891	-0.783	26.903 26.760	1.00	0.00	3A4 3A4
ATOM	226	CD	GLN	77 77	15.977 16.121	-1.843 -2.718	27.611	1.00	0.00	3A4
ATOM ATOM	227 228		GLN GLN	77	16.759	-1.765	25.648	1.00	0.00	3A4
ATOM	229	C	GLN	77	12.593	0.983	27.782	1.00	0.00	3A4
ATOM	230	ŏ	GLN	77	12.935	1.504	26.719	1.00	0.00	3A4
ATOM	231	N	GLN	78	12.365	1.707	28.918	1.00	0.00	3A4
ATOM	232	CA	GLN	78	12.698	3.105	29.188	1.00	0.00	3A4
ATOM	233	СВ	GLN	78	14.220	3.411	28.944	1.00	0.00	3A4
MOTA	234	CG	GLN	78	14.774	4.789	29.381	1.00	0.00	3A4
MOTA	235	CD	GLN	78	14.622	5.043	30.889		0.00	3A4
ATOM	236		GLN	78 70	14.409	4.138	31.694 31.296		0.00	3A4 3A4
ATOM ATOM	237 238		GLN	78 78	14.757 11.820	6.336 4.135	28.453		0.00	3A4
ATOM ATOM	238	С О	GLN GLN	78	11.794	4.125	27.222		0.00	3A4
ATOM	240	N	PRO	79	11.120	5.089	29.129			3A4
ATOM	241	CA	PRO	79	10.604	6.330	28.550			3A4
ATOM	242	CD	PRO	79	10.730	4.946	30.533	1.00	0.00	3A4
MOTA	243	СВ	PRO	79	9.535	6.798	29.557			3A4
MOTA	244	CG	PRO	79	10.001	6.244	30.911			3A4
ATOM	245	С	PRO	79	11.734	7.327	28.383	1.00	0.00	3A4

ATOM	246	0	PRO	79	12.582	7.447	29.260	1.00	0.00	3A4
ATOM	247	N	VAL	80	11.782	8.012	27.228	1.00	0.00	3A4
ATOM	248	CA	VAL	80	12.870	8.876	26.835	1.00	0.00	3A4
ATOM	249	СВ	VAL	80	13.698	8.283	25.679	1.00	0.00	3A4 3A4
ATOM	250	CG1 CG2		80	14.441 12.828	7.026 7.928	26.173 24.440	1.00	0.00	3A4
ATOM ATOM	251 252	CGZ	VAL VAL	80 80	12.020	10.173	26.392	1.00	0.00	3A4
ATOM	253	Ö	VAL	80	11.117	10.204	25.939	1.00	0.00	3A4
ATOM	254	N	LEU	81	13.003	11.285	26.466	1.00	0.00	3A4
ATOM	255	CA	LEU	81	12.603	12.575	25.948	1.00	0.00	3A4
ATOM	256	CB	LEU	81	12.958	13.700	26.945	1.00	0.00	3A4
MOTA	257	CG	LEU	81	12.302	15.079	26.699	1.00	0.00	3A4
ATOM	258		LEU	81	10.822	15.078 16.197	27.116 27.437	1.00	0.00	3A4 3A4
ATOM ATOM	259 260	CD2	LEU	81 81	13.057 13.352	12.751	24.647	1.00	0.00	3A4
ATOM	261	ŏ	LEU	81	14.529	12.427	24.569	1.00	0.00	3A4
ATOM	262	N	ALA	82	12.695	13.249	23.585	1.00	0.00	3A4
ATOM	263	CA	ALA	82	13.260	13.415	22.267	1.00	0.00	3A4
ATOM	264	CB	ALA	82	12.433	12.689	21.183	1.00	0.00	3A4
MOTA	265	С	ALA	82	13.288	14.890	21.990	1.00	0.00	3A4 3A4
MOTA	266	0	ALA	82	12.251	15.546 15.436	22.002 21.733	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	267 268	N CA	ILE ILE	83 83	14.498 14.742	16.837	21.486	1.00	0.00	3A4
ATOM	269	CB	ILE	83	16.032	17.330	22.124	1.00	0.00	3A4
ATOM	270	CG2	ILE	83	15.944	18.846	22.217	1.00	0.00	3A4
ATOM	271	CG1	ILE	83	16.359	16.727	23.506	1.00	0.00	3A4
MOTA	272	CD	ILE	83	15.380	17.044	24.634	1.00	0.00	3A4
ATOM	273	C	ILE	83	14.831	17.000	19.986	1.00	0.00	3A4 3A4
ATOM	274 275	O N	ILE	83 84	15.706 13.915	16.418 17.773	19.358 19.367	$1.00 \\ 1.00$	0.00	3A4
ATOM ATOM	276	CA	THR THR	84	13.796	17.851	17.920	1.00	0.00	3A4
ATOM	277	СВ	THR	84	12.384	17.503	17.457	1.00	0.00	3A4
MOTA	278	OG1	THR	84	11.371	18.330	18.025	1.00	0.00	3A4
ATOM	279	CG2		84	12.085	16.027	17.808	1.00	0.00	3A4
ATOM	280	C	THR	84	14.259	19.175	17.344	1.00	0.00	3A4 3A4
ATOM	281 282	O N	THR ASP	84 85	14.500 14.371	19.282 20.231	16.144 18.176	1.00	0.00	3A4
ATOM ATOM	283	CA	ASP	85	14.595	21.594	17.732	1.00	0.00	3A4
ATOM	284	СВ	ASP	85	13.703	22.550	18.577	1.00	0.00	3A4
ATOM	285	CG	ASP	85	13.371	23.873	17.872	1.00	0.00	3A4
ATOM	286		ASP	85	12.666	23.828	16.828	1.00	0.00	3A4
ATOM	287	OD2		85 85	13.808 16.050	24.942 21.928	18.373 17.888	1.00	0.00	3A4 3A4
ATOM ATOM	288 289	С 0	ASP ASP	85 85	16.660	21.452	18.843	1.00	0.00	3A4
ATOM	290	N	PRO	86	16.683	22.732	17.024	1.00	0.00	3A4
ATOM	291	CA	PRO	86	18.101	23.035	17.076	1.00	0.00	3A4
ATOM	292	CD	PRO	86	16.102	23.257	15.807	1.00	0.00	3A4
MOTA	293	CB	PRO	86	18.421	23.751	15.747	1.00	0.00	3A4 3A4
ATOM	294 295	CG	PRO PRO	86 86	17.079 18.425	24.309 23.863	15.294 _. 18.284	1.00	0.00	3A4
ATOM ATOM	296	Ö	PRO	86	19.466	23.647	18.892	1.00	0.00	3A4
ATOM	297	N	ASP	87	17.511			1.00	0.00	3A4
ATOM	298	CA	ASP	87	17.636	25.559	19.902	1.00	0.00	3A4
ATOM	299	СВ	ASP	87	16.417	26.494	20.029	1.00	0.00	3A4
ATOM	300	CG	ASP	87	16.305	27.442	18.820 18.258	1.00	0.00	3A4 3A4
ATOM ATOM	301 302		ASP	87 87	17.357 15.148	27.851 27.764	18.439	1.00	0.00	3A4
ATOM	303	C	ASP	87	17.724	24.745	21.171	1.00	0.00	3A4
ATOM	304	Ō	ASP	87	18.546	25.018	22.032	1.00	0.00	3A4
ATOM	305	N	MET	88	16.902	23.678	21.253	1.00	0.00	3A4
ATOM	306	CA	MET	88	16.847	22.776	22.375	1.00	0.00	3A4
ATOM	307	CB	MET	88	15.536	22.000	22.396 22.644	1.00	0.00	3A4 3A4
MOTA MOTA	308 309	CG SD	MET MET	88 88	14.362	22.948 22.177	23.469		0.00	3A4
ATOM	310	CE	MET	88	13.722	21.914	25.087		0.00	3A4
ATOM	311	č	MET	88	18.007	21.812	22.436		0.00	3A4
ATOM	312	0	MET	88	18.524	21.506			0.00	3A4
ATOM	313	N	ILE	89	18.500	21.349	21.264		0.00	3A4
ATOM	314	CA	ILE		19.637	20.450			0.00	3A4 3A4
ATOM ATOM	315 316	CB CG2	ILE		19.679 21.088	19.800 19.217			0.00	3A4
ATOM	317		ILE		18.596	18.681	19.910		0.00	3A4
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ATOM	318	CD	ILE	89	18.390	17.678	18.773	1.00	0.00	3A4
MOTA	319	С	ILE	89	20.916	21.161	21.538	1.00	0.00	3A4
ATOM	320	0	ILE	89	21.722	20.655	22.310	1.00	0.00	3A4
ATOM	321	N	LYS	90	21.096	22.421	21.089	1.00	0.00	3A4
MOTA	322	CA	LYS	90	22.214	23.250	21.481	1.00	0.00	3A4
MOTA	323	СВ	LYS	90	22.225	24.577	20.719	1.00	0.00	3A4
MOTA	324	CG	LYS	90	23.531	25.387	20.790	1.00	0.00	3A4
ATOM	325	CD	LYS	90	23.546	26.569	19.811	1.00	0.00	3A4
ATOM	326	CE	LYS	90	24.875	27.339	19.774	1.00	0.00	3A4
ATOM	327	NZ	LYS	90	25.167	27.975	21.082	1.00	0.00	3A4
MOTA	328	С	LYS	90	22.221	23.564	22.961	1.00	0.00	3A4
MOTA	329	0	LYS	90	23.248	23.567	23.612	1.00	0.00	3A4
ATOM	330	N	THR	91	21.031	23.752	23.561	1.00	0.00	3A4
MOTA	331	CA	THR	91	20.855	23.981	24.981	1.00	0.00	3A4
ATOM	332	CB	THR	91	19.434	24.380	25.293	1.00	0.00	3A4
ATOM	333	OG1	THR	91	19.170	25.637	24.681	1.00	0.00	3A4
ATOM	334	CG2	THR	91	19.109	24.554	26.810	1.00	0.00	3A4
ATOM	335	С	THR	91	21.198	22.782	25.817	1.00	0.00	3A4
MOTA	336	0	THR	91	21.850	22.889	26.851	1.00	0.00	3A4
ATOM	337	N	VAL	92	20.849	21.578	25.307	1.00	0.00	3A4
ATOM	338	CA	VAL	92	21.125	20.315	25.945	1.00	0.00	3A4
MOTA	339	СВ	VAL	92	20.299	19.178	25.353	1.00	0.00	3A4
MOTA	340		VAL	92	21.025	18.247	24.370	1.00	0.00	3A4
MOTA	341	CG2	VAL	92	19.643	18.370	26.498	1.00	0.00	3A4
MOTA	342	С	VAL	92	22.600	20.047	26.089	1.00	0.00	3A4
MOTA	343	0	VAL	92	22.991	19.412	27.041	1.00	0.00	3A4
ATOM	344	N	LEU	93	23.483	20.706	25.311	1.00	0.00	3A4
MOTA	345	CA	LEU	93	24.914	20.851	25.543	1.00	0.00	3A4
ATOM	346	СВ	LEU	93	25.432	21.742	24.407	1.00	0.00	3A4
ATOM	347	CG	LEU	93	26.456	21.108	23.525	1.00	0.00	3A4 3A4
MOTA	348		LEU	93	25.796	19.892	22.820	1.00	0.00	3A4
ATOM	349		LEU	93	26.955	22.238	22.601	1.00	0.00	3A4
ATOM	350	С	LEU	93	25.419	21.473	26.847	1.00	0.00	3A4
ATOM	351	0	LEU	93	24.654	21.997	27.655	1.00	0.00	3A4
ATOM	352	N	VAL	94	26.774	21.385	27.035	1.00	0.00	3A4
ATOM	353	CA	VAL	94	27.599	21.729 23.082	28.196 28.879	1.00	0.00	3A4
ATOM	354	CB	VAL	94	27.328			1.00	0.00	3A4
ATOM	355		VAL	94	28.368	23.358 24.201	30.001 27.813	1.00	0.00	3A4
ATOM	356		VAL	94 94	27.427 27.515	20.540	29.137	1.00	0.00	3A4
ATOM	357 358	С О	VAL VAL	94	26.875	20.578	30.188	1.00	0.00	3A4
ATOM	359	N	LYS	95	28.141	19.421	28.690	1.00	0.00	3A4
ATOM ATOM	360	CA	LYS	95	28.019	18.101	29.261	1.00	0.00	3A4
ATOM	361	CB	LYS	95	27.404	17.078	28.259	1.00	0.00	3A4
ATOM	362	CG	LYS	95	27.757	17.284	26.778	1.00	0.00	3A4
ATOM	363	CD	LYS	95	27.133	16.199	25.898	1.00	0.00	3A4
ATOM	364	CE	LYS	95	27.017	16.559	24.413	1.00	0.00	3A4
ATOM	365	NZ	LYS	95	28.338	16.819	23.809	1.00	0.00	3A4
ATOM	366	c	LYS	95	29.379	17.675	29.736	1.00	0.00	3 <u>A</u> 4
ATOM	367	o	LYS	95	30.123	16.990	29.040	1.00	0.00	3A4
ATOM	368	N	GLU	96	29.703	18.085	30.988	1.00	0.00	3A4
ATOM	369	CA	GLU	96	30.926	17.783	31.698	1.00	0.00	3A4
ATOM	370.	СВ	GLU	96	31.795	19.051	31.950	1.00	0.00	3A4
ATOM	371	CG	GLU	96	31.039	20.290	32.48.6	1.00	0.00	3A4
ATOM	372	CD	GLU	96	32.012	21.467	32.599	1.00	0.00	3A4
ATOM	373	OE1	GLU	96	31.790	22.493	31.901	1.00	0.00	3A4
ATOM	374	OE2	GLU	96	32.990	21.357	33.388	1.00	0.00	3A4
ATOM	375	С	GLU	96	30.517	17.078	32.969	1.00	0.00	3A4
ATOM	376	0	GLU	96	30.732	17.576	34.073	1.00	0.00	3A4
MOTA	377	N	CYS	97	29.924	15.869	32.763	1.00	0.00	3A4
ATOM	378	CA	CYS	97	29.436	14.865	33.693		0.00	3A4
MOTA	379	CB	CYS	97	29.558	15.141	35.235		0.00	3A4
MOTA	380	SG	CYS	97	29.186	13.706	36.313		0.00	3A4
ATOM	381	С	CYS	97	28.000	14.633	33.277		0.00	3A4
MOTA	382	0	CYS	97	27.076	15.253	33.800		0.00	3A4
MOTA	383	N	TYR	98	27.817	13.703	32.305		0.00	3A4
ATOM	384	CA	TYR	98	26.556	13.216	31.782		0.00	3A4
MOTA	385	СВ	TYR	98	26.197	13.814	30.380		0.00	3A4
MOTA	386	CG	TYR	98	25.205	14.939	30.543		0.00	3A4
MOTA	387		TYR	98	25.573	16.198	31.050		0.00	3A4
MOTA	388		TYR	_	23.862	14.731	30.197		0.00	3A4
ATOM	389	CE:	TYR	98	24.626	17.224	31.198	1.00	0.00	3A4

ATOM	390	CE2	TYR	98	22.901	15.740	30.351	1.00	0.00	3A4
ATOM	391	CZ	TYR	98	23.286	16.993	30.849	1.00	0.00	3A4
ATOM	392	OH	TYR	98	22.323	18.015	30.999	1.00	0.00	3A4
ATOM	393	С	TYR	98	26.800	11.735	31.683	1.00	0.00	3A4
MOTA	394	0	TYR	98	27.629	11.292	30.891	1.00	0.00	3A4
ATOM	395	N	SER	99	26.097	10.928	32.531	1.00	0.00	3A4
MOTA	396	CA	SER	99	26.414	9.536	32.838	1.00	0.00	3A4 3A4
ATOM	397	СВ	SER	99	25.870	9.141	34.247	1.00	0.00	3A4
ATOM	398	OG	SER	99	26.515 25.931	7.992 8.568	34.791 31.771	1.00	0.00	3A4
ATOM	399	c o	SER SER	99 99	24.885	8.764	31.156	1.00	0.00	3A4
ATOM ATOM	400 401	N	VAL	100	26.759	7.507	31.524	1.00	0.00	3A4
ATOM	402	CA	VAL	100	26.647	6.426	30.542	1.00	0.00	3A4
ATOM	403	CB	VAL	100	25.344	5.612	30.576	1.00	0.00	3A4
ATOM	404		VAL	100	25.483	4.356	29.677	1.00	0.00	3A4
ATOM	405	CG2	VAL	100	25.062	5.167	32.031	1.00	0.00	3A4
ATOM	406	С	VAL	100	26.977	6.962	29.152	1.00	0.00	3A4
ATOM	407	0	VAL	100	28.088	6.758	28.673	1.00	0.00	3A4
MOTA	408	N	PHE	101	26.002	7.682	28.517	1.00	0.00	3A4
MOTA	409	CA	PHE	101	26.131	8.581	27.372	1.00	0.00	3A4 3A4
ATOM	410	CB	PHE	101	27.487 27.503	9.383 10.546	27.359 26.402	1.00	0.00 0.00	3A4
ATOM	411	CG	PHE	101 101	26.587	11.609	26.522	1.00	0.00	3A4
ATOM ATOM	412 413		PHE PHE	101	28.432	10.563	25.350	1.00	0.00	3A4
ATOM	414		PHE	101	26.580	12.640	25.573	1.00	0.00	3A4
ATOM	415		PHE	101	28.435	11.597	24.418	1.00	0.00	3A4
ATOM	416	cz	PHE	101	27.492	12.629	24.516	1.00	0.00	3A4
ATOM	417	Ċ	PHE	101	25.860	7.863	26.049	1.00	0.00	3A4
ATOM	418	0	PHE	101	25.613	8.506	25.030	1.00	0.00	3A4
ATOM	419	N	THR	102	25.881	6.507	26.048	1.00	0.00	3A4
MOTA	420	CA	THR	102	25.468	5.674	24.939	1.00	0.00	3A4
ATOM	421	CB	THR	102	26.561	5.456	23.875	1.00	0.00	3A4 3A4
ATOM	422		THR	102	26.134	4.618	22.803	1.00	0.00	3A4
ATOM	423	CG2		102	27.920	4.971 4.448	24.441 25.660	1.00	0.00	3A4
ATOM	424	C O	THR	102 102	24.949 25.680	3.511	25.976	1.00	0.00	3A4
ATOM ATOM	425 426	N	THR ASN	102	23.629	4.491	25.991	1.00	0.00	3A4
ATOM	427	CA	ASN	103	22.973	3.634	26.965	1.00	0.00	3A4
ATOM	428	СВ	ASN	103	22.145	4.482	28.000	1.00	0.00	3A4
ATOM	429	CG	ASN	103	21.193	5.519	27.373	1.00	0.00	3A4
ATOM	430	OD1	ASN	103	21.530	6.702	27.345	1.00	0.00	3A4
MOTA	431		ASN	103	19.993	5.093	26.893	1.00	0.00	3A4
MOTA	432	С	ASN	103	22.171	2.529	26.295	1.00	0.00	3A4 3A4
MOTA	433	0	ASN	103	22.526	2.061	25.214	1.00	0.00 0.00	3A4
ATOM	434	N	ARG	104	21.099 20.255	0.904	27.018 26.922	1.00	0.00	3A4
ATOM ATOM	435 436	CA CB	ARG ARG	104 104	20.253	0.305	25.521	1.00	0.00	3A4
ATOM	437	CG	ARG	104	19.266	1.224	24.571	1.00	0.00	3A4
ATOM	438	CD	ARG	104	19.318		23.096	1.00	0.00	. 3A4
ATOM	439	NE	ARG	104	20.722	1.001	22.589	1.00	0.00	3A4
MOTA	440	CZ	ARG	104	21.086	0.812	21.280	1.00	0.00	3A4
MOTA	441	NH1	ARG	104	22.383	1.027				3A4
MOTA	442		ARG	104	20.184	0.403	20.340	1.00	0.00	3A4
ATOM	443	C	ARG	104	20.801	-0.116	27.892	1.00	0.00	3A4 3A4
ATOM	444	0	ARG	104	21.996	-0.173	28.177	1.00	0.00 0.00	3A4
ATOM	445	N	ARG	105	19.899 20.180	-0.953 -1.924	28.439 29.470		0.00	3A4
ATOM ATOM	446 447	CA CB	ARG ARG	105 105	18.917	-2.306	30.269		0.00	3A4
ATOM	448	CG	ARG	105	18.288	-1.109			0.00	3A4
MOTA	449	CD	ARG	105	17.273	-0.267	30.201		0.00	3A4
ATOM	450	NE	ARG	105	16.999	1.019	30.940		0.00	3A4
ATOM	451	CZ	ARG	105	17.736	2.168	30.769	1.00	0.00	3A4
ATOM	452		ARG	105	17.471	3.253			0.00	3A4
ATOM	453	NH2	? ARG	105	18.734	2.262			0.00	3A4
ATOM	454	С	ARG	105	20.851	-3.183				3A4
ATOM	455	0	ARG		21.862	-3.545				3A4 3A4
ATOM	456	N	PRO		20.439	-3.879 -5.066				3A4 3A4
ATOM	457	CA	PRO		21.118 19.166	-3.707				3A4
MOTA MOTA	458 459	CD CB	PRO PRO		20.292	-5.535				3A4
ATOM	460	CG	PRO		19.354	-4.383				3A4
MOTA	461	C	PRO		22.531	-4.785				3A4
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ATOM	462	0	PRO	106	23.412	-5.580	27.239	1.00	0.00	3A4
ATOM	463	N	PHE	107	22.789	-3.612	26.347	1.00	0.00	3A4
ATOM	464	CA	PHE	107	24.092	-3.149	25.939	1.00	0.00	3A4
ATOM	465	СВ	PHE	107	23.996	-1.854	25.067	1.00	0.00	3A4
ATOM	466	CG	PHE	107		-2.185	23.730	1.00	0.00	3A4
ATOM	467		PHE	107	24.194	-2.404	22.604	1.00	0.00	3A4 3A4
ATOM	468		PHE	107	21.982	-2.301	23.578 21.360	1.00	0.00	3A4
ATOM	469		PHE	107 107	23.633 21.415	-2.730 -2.640	22.342	1.00	0.00	3A4
ATOM	470 471	CZ	PHE PHE	107	22.243	-2.850	21.231	1.00	0.00	3A4
ATOM ATOM	472	C	PHE	107	24.996	-2.874	27.117	1.00	0.00	3A4
ATOM	473	ŏ	PHE	107	26.183	-3.178	27.071	1.00	0.00	3A4
ATOM	474	N	GLY	108	24.445	-2.352	28.235	1.00	0.00	3A4
ATOM	475	CA	GLY	108	25.169	-2.115	29.465	1.00	0.00	3A4
ATOM	476	С	GLY	108	25.703	-3.372	30.122	1.00	0.00	3A4
ATOM	477	0	GLY	108	26.825	-3.365	30.623	1.00	0.00	3A4
ATOM	478	N	PRO	109	24.957	-4.476	30.112	1.00	0.00	3A4
ATOM	479	CA	PRO	109	25.476	-5.825	30.348	1.00	0.00	3A4
MOTA	480	CD	PRO	109	24.065	-4.305	31.286	1.00	0.00 0.00	3A4 3A4
ATOM	481	CB	PRO	109	24.191	-6.637 -5.658	30.615 31.433	1.00 1.00	0.00	3A4
ATOM	482	CG	PRO	109 109	23.330 26.330	-6.541	29.318	1.00	0.00	3A4
ATOM ATOM	483 484	C C	PRO PRO	109	27.456	-6.908	29.658	1.00	0.00	3A4
ATOM	485	N	VAL	110	25.774	-6.864	28.119	1.00	0.00	3A4
ATOM	486	CA	VAL	110	26.331	-7.778	27.133	1.00	0.00	3A4
ATOM	487	СВ	VAL	110	25.389	-8.936	26.768	1.00	0.00	3A4
ATOM	488		VAL	110	25.412	-9.943	27.938	1.00	0.00	3A4
ATOM	489	CG2	VAL	110	23.943	-8.492	26.450	1.00	0.00	3A4
ATOM	490	С	VAL	110	26.744	-6.971	25.923	1.00	0.00	3A4
MOTA	491	0	VAL	110	25.981	-6.165	25.392	1.00	0.00	3A4
ATOM	492	N	GLY	111	28.021	-7.174	25.497	1.00	0.00	3A4 3A4
ATOM	493	CA	GLY	111	28.732	-6.403	24.496 25.245	1.00	0.00 0.00	3A4
ATOM	494	C	GLY	111 111	29.773 29.468	-5.622 -4.588	25.839	1.00	0.00	3A4
ATOM	495 496	O N	GLY PHE	112	31.035	-6.136	25.266	1.00	0.00	3A4
ATOM ATOM	497	CA	PHE	112	32.105	-5.711	26.158	1.00	0.00	3A4
ATOM	498	СВ	PHE	112	32.907	-6.929	26.720	1.00	0.00	3A4
ATOM	499	CG	PHE	112	31.979	-7.800	27.529	1.00	0.00	3A4
ATOM	500		PHE	112	31.631	-9.095	27.096	1.00	0.00	3A4
ATOM	501	CD2	PHE	112	31.424	-7.318	28.732	1.00	0.00	3A4
MOTA	502		PHE	112	30.746	-9.883	27.847	1.00	0.00	3A4
MOTA	503		PHE	112	30.537	-8.104	29.480	1.00	0.00	3A4 3A4
ATOM	504	CZ	SHE	112	30.195	-9.387	29.035	1.00	0.00	3A4
ATOM	505	C	PHE	112	33.050 34.190	-4.749 -5.078	25.472 25.148	1.00	0.00	3A4
ATOM ATOM	506 507	O N	PHE	112 113	32.562	-3.489	25.295	1.00	0.00	3A4
ATOM	508	CA	MET	113	33.296	-2.314	24.869	1.00	0.00	3A4
ATOM	509	СВ	MET	113	32.602	-1.505	23.728	1.00	0.00	3A4
ATOM	510	CG	MET	113	32.554	-2.210	22.356	1.00	.0.00	3A4
ATOM	511	SD	MET	113	31.429	-3.639	22.184	1.00	0.00	3A4
ATOM	512	CE	MET	113	29.851	-2.787	22.471	1.00	0.00	3A4
ATOM	513	С	MET	113	33.386	-1.481	26.125	1.00	0.00	3A4
MOTA	514	0	MET	113	32.371	-1.027	26.652	1.00	0.00	3A4
MOTA	515	N	LYS	114	34.630	-1.321	26.660	1.00	0.00	3A4 3A4
MOTA	516	CA	LYS	114	34.932 36.207	-0.910 -1.643	28.025 28.544	1.00	0.00 0.00	3A4
ATOM ATOM	517 518	CB CG	LYS LYS	114 114	36.129	-3.170	28.392	1.00		3A4
ATOM	519	CD	LYS	114	37.411	-3.890	28.832	1.00		3A4
ATOM	520	CE	LYS	114	37.355	-5.417	28.667			3A4
ATOM	521	NZ	LYS	114	37.190	-5.806	27.244	1.00		3A4
ATOM	522	c	LYS	114	35.074	0.600	28.136	1.00	0.00	3A4
ATOM	523	0	LYS	114	34.485	1.339	27.348			3A4
MOTA	524	N	SER	115	35.857	1.092	29.141			3A4
MOTA	525	CA	SER	115	35.955	2.486				3A4
MOTA	526	СВ	SER	115	36.419	2.597	31.048			3A4
ATOM	527	OG	SER	115	35.505	1.921	31.901			3A4 3A4
ATOM	528	C	SER		36.891	3.307				3A4 3A4
ATOM	529	O N	SER		38.106 36.300	3.302 4.041				3A4
ATOM ATOM	530 531	N CA	ALA ALA	116 116	36.990	4.902				3A4
ATOM	532	CB	ALA		36.806	4.440				3A4
ATOM	533	C	ALA		36.445	6.277				3A4
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MOTA	534	0	ALA	116	35.934	6.634			0.00 0.00	3A4 3A4
ATOM	535	И	ILE	117 117	36.498 36.054	7.116 8.497	25.886 25.985	_	0.00	3A4
ATOM ATOM	536 537	CA CB	ILE	117	36.818	9.363	24.999	1.00	0.00	3A4
ATOM	538	CG2		117	36.637	8.922	23.524	1.00	0.00	3A4
ATOM	539		ILE	117		10.857	25.212	1.00	0.00	3A4 3A4
MOTA	540	CD	ILE	117	37.122 34.556	11.262 8.659	26.574 25.822	1.00	0.00 0.00	3A4
ATOM ATOM	541 542	С 0	ILE	117 117	33.924	9.474	26.492	1.00	0.00	3A4
ATOM	543	N	SER	118	33.923	7.843	24.946	1.00	0.00	3A4
ATOM	544	CA	SER	118	32.533	8.033	24.588	1.00	0.00	3A4 3A4
MOTA	545	СВ	SER	118	32.205 32.499	7.525 6.147	23.146 22.946	1.00	0.00	3A4
ATOM ATOM	546 547	OG C	SER SER	118 118	31.585	7.455	25.606	1.00	0.00	3A4
ATOM	548	ŏ	SER	118	30.395	7.686	25.524	1.00	0.00	3A4
ATOM	549	N	ILE	119	32.084	6.735	26.630	1.00	0.00	3A4
MOTA	550	CA	ILE	119	31.251	6.157	27.657	1.00	0.00	3A4 3A4
MOTA	551	CB	ILE ILE	119 119	31.480 32.895	4.637 4.296	27.705 28.225	1.00	0.00	3A4
ATOM ATOM	552 553		ILE	119	30.373	3.794	28.400	1.00	0.00	3A4
ATOM	554	CD	ILE	119	29.071	3.681	27.605	1.00	0.00	3A4
ATOM	555	C	ILE	119	31.475	6.827	29.005	1.00	0.00	3A4 3A4
MOTA	556	0	ILE	119	30.894	6.426	30.013 29.050	1.00	0.00 0.00	3A4
ATOM	557 558	N CA	ALA ALA	120 120	32.350 32.876	7.862 8.420	30.276	1.00	0.00	3A4
ATOM ATOM	559	CB	ALA	120	34.429	8.417	30.275	1.00	0.00	3A4
ATOM	560	c	ALA	120	32.403	9.821	30.537	1.00	0.00	3A4
MOTA	561	0	ALA	120	32.153	10.624	29.642	1.00	0.00	3A4 3A4
ATOM	562	N	GLU	121	32.338 31.987	10.132 11.402	31.847 32.421	1.00	0.00 0.00	3A4
ATOM ATOM	563 564	CA CB	GLU GLU	121 121	31.189	11.213	33.742	1.00	0.00	3A4
ATOM	565	CG	GLU	121	29.884	10.420	33.613	1.00	0.00	3A4
ATOM	566	CD	GLU	121	30.124	8.902	33.618	1.00	0.00	3A4
MOTA	567		GLU	121	29.800	8.241	32.594 34.649	1.00	0.00	3A4 3A4
ATOM	568	OE2	GLU	121 121	30.631 33.282	8.385 12.104	32.738	1.00	0.00	3A4
ATOM ATOM	569 570	Ö	GLU	121	34.307	11.460	32.947	1.00	0.00	3A4
ATOM	571	N	ASP	122	33.267	13.450	32.868	1.00	0.00	3A4
ATOM	572	CA	ASP	122	34.366	14.255	33.384	1.00	0.00	3A4 3A4
ATOM	573	CB CG	ASP ASP	122 122	33.940 35.057	15.762 16.786	33.320 33.606	1.00	0.00	3A4
ATOM ATOM	574 575		ASP	122	34.911	17.556	34.593	1.00	0.00	3A4
ATOM	576		ASP	122	36.057	16.817	32.842	1.00	0.00	3A4
ATOM	577	С	ASP	122	34.615	13.879	34.870	1.00	0.00	3A4 3A4
ATOM	578	0	ASP	122 123	33.636 35.863	13.610 13.792	35.566 35.421	1.00	0.00	3A4
MOTA MOTA	579 580	N CA	GLU GLU	123	37.162	14.248	34.972	1.00	0.00	3A4
ATOM	581	СВ	GLU	123	37.993	14.687	36.197	1.00	0.00	3A4
ATOM	582	CG	GLU	123	37.348	15.854	36.968		0.00	3A4 3A4
MOTA	583	CD	GLU	123	38.253 38.764	16.265 17.417	38.134 38.116	1.00	0.00	3A4
MOTA MOTA	584 585		GLU GLU	123 123	38.443	15.431		1.00	0.00	3A4
MOTA	586	c	GLU	123	37.950	13.205		1.00		3A4
MOTA	587	0	GLU	123	39.000	13.494		1.00		3A4 3A4
MOTA	588	N	GLU	124	37.449 38.063	11.951 10.827				3A4
MOTA MOTA	589 590	CA CB	GLU GLU	124 124	37.284	9.523				3A4
ATOM	591	CG	GLU	124	37.186	9.213				3A4
MOTA	592	CD	GLU	124	36.410	7.908				3A4
ATOM	593		1 GLU	124	37.010	6.933 7.870			_	3A4 3A4
ATOM	594 595		GLU GLU	124 124	35.204 38.109	11.000				3A4
ATOM ATOM	596		GLU	124	39.087	10.727		1.00	0.00	3A4
ATOM	597	N	TRP	125	37.027	11.579				3A4
ATOM	598		TRP	125	36.896	11.901				3A4 3A4
ATOM	599		TRP TRP	125 125	35.456 35.096	12.317 13.136				3A4
ATOM ATOM	600 601		TRP 2 TRP		34.736	14.501				3A4
ATOM	602	CD	1 TRP	125	34.423	12.765	27.428	1.00		3A4
ATOM	603		1 TRP		33.701	13.815				3A4 3A4
MOTA	604		2 TRP		33.805 35.040	14.860 15.361				3A4
MOTA	605	CE	3 TRP	123	33.040	13.50	. 23.07			

ATOM	606	ÇZ2	TRP	125	33.124	16.059	27.921	1.00	0.00	3A4
ATOM	607	CZ3	TRP	125	34.396	16.599	29.921	1.00	0.00	3A4
ATOM	608	CH2		125	33.421	16.924	28.984	1.00	0.00	3A4 3A4
ATOM	609 610	C O	TRP TRP	125 125	37.893 38.564	12.940 12.734	29.585 28.590	1.00	0.00	3A4
ATOM ATOM	611	N	LYS	126	38.066	14.068	30.315	1.00	0.00	3A4
ATOM	612	CA	LYS	126	38.948	15.161	29.915	1.00	0.00	3A4
ATOM	613	СВ	LYS	126	38.776	16.362	30.855	1.00	0.00	3A4
MOTA	614	CG	LYS	126	39.424	17.682	30.406	1.00	0.00	3A4
MOTA	615	CD	LYS	126	39.026	18.858	31.300	1.00 1.00	0.00	3A4 3A4
ATOM	616 617	CE NZ	LYS LYS	126 126	39.634 39.206	20.191 21.296	30.845 31.735	1.00	0.00	3A4
ATOM ATOM	618	C	LYS	126	40.413	14.775	29.867	1.00	0.00	3A4
ATOM	619	ō	LYS	126	41.152	15.173	28.977	1.00	0.00	3A4
MOTA	620	N	ARG	127	40.830	13.884	30.785	1.00	0.00	3A4
MOTA	621	CA	ARG	127	42.152	13.315	30.821	1.00	0.00	3A4
ATOM	622	CB	ARG	127	42.369 42.319	12.556 13.460	32.148 33.385	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	623 624	CG CD	ARG ARG	127 127	42.230	12.652	34.686	1.00	0.00	3A4
ATOM	625	NE	ARG	127	42.079	13.613	35.835	1.00	0.00	3A4
ATOM	626	CZ	ARG	127	41.521	13.267	37.040	1.00	0.00	3A4
ATOM	627	NH1	ARG	127	41.438	14.206	38.026	1.00	0.00	3A4
MOTA	628		ARG	127	41.040	12.009	37.276	1.00	0.00	3A4 3A4
MOTA	629	C	ARG	127	42.448 43.503	12.378 12.464	29.678 29.060	1.00	0.00 0.00	3A4
ATOM ATOM	630 631	O N	ARG LEU	127 128	41.487	11.489	29.329	1.00	0.00	3A4
ATOM	632	CA	LEU	128	41.614	10.553	28.227	1.00	0.00	3A4
ATOM	633	СВ	LEU	128	40.552	9.436	28.305	1.00	0.00	3A4
MOTA	634	CG	LEU	128	40.710	8.475	29.510	1.00	0.00	3A4
ATOM	635		LEU	128	39.492	7.536 7.670	29.620 29.503	1.00	0.00	3A4 3A4
ATOM ATOM	636 637	CD2	LEU	128 128	42.026 41.513	11.260	26.900	1.00	0.00	3A4
ATOM	638	ŏ	LEU	128	42.307	10.998	26.016	1.00	0.00	3A4
ATOM	639	N	λRG	129	40.613	12.256	26.764	1.00	0.00	3A4
MOTA	640	CA	ARG	129	40.455	13.056	25.570	1.00	0.00	3A4
ATOM	641	CB	ARG	129	39.248	13.995	25.706	1.00	0.00	3A4 3A4
ATOM	642 643	CG CD	ARG ARG	129 129	38.865 37.443	14.698 15.285	24.411 24.477	1.00	0.00	3A4
ATOM ATOM	644	NE	ARG	129	36.965	15.632	23.089	1.00	0.00	3A4
ATOM	645	CZ	ARG	129	37.094	16.870	22.512	1.00	0.00	3A4
ATOM	646	NH1	ARG	129	36.589	17.069	21.260	1.00	0.00	3A4
MOTA	647		ARG	129	37.709	17.907	23.155	1.00	0.00	3A4 3A4
ATOM	648	c	ARG	129 129	41.673 42.125	13.896 13.963	25.247 24.109	1.00	0.00	3A4
ATOM ATOM	649 650	О И	ARG SER	130	42.292	14.491	26.294	1.00	0.00	3A4
ATOM	651	CA	SER	130	43.486	15.299	26.191	1.00	0.00	3A4
ATOM	652	CB	SER	130	43.870	16.030	27.515	1.00	0.00	3A4
ATOM	653	OG	SER	130	42.925	17.049	27.812	1.00	0.00	3A4 3A4
ATOM	654	c	ŞER SER	130 130	44.691 45.506	14.547 15.121	25.703 25.002	1.00	0.00	3A4
ATOM ATOM	655 656	O N	LEU	131	44.822	13.241	26.004	1.00	0.00	3A4
ATOM	657	CA	LEU	131	45.894	12.396		1.00	0.00	3A4
MOTA	658	CB	LEU	131	45.835	11.013	26.195	1.00	0.00	3A4
ATOM	659	CG	LEU	131	46.473	11.008	27.591	1.00	0.00	3A4
ATOM	660		LEU	131 131	45.836 48.005	9.924 10.845	28.474 27.482	1.00	0.00	3A4 3A4
ATOM ATOM	661 662	CDZ	LEU LEU	131	45.875	12.189	24.006	1.00	0.00	3A4
ATOM	663	ŏ	LEU	131	46.913	12.177	23.361	1.00	0.00	3A4
MOTA	664	N	LEU	132	44.675	12.059	23.421	1.00	0.00	3A4
ATOM	665	CA	LEU	132	44.436	11.692	22.040	1.00	0.00	3A4
ATOM	666	CB	LEU	132	43.113	10.883	21.884 23.187	1.00	0.00	3A4 3A4
ATOM ATOM	667 668	CG	LEU LEU	132 132	42.628 41.170	10.220 9.739	23.187	1.00	0.00	3A4
ATOM	669		LEU	132	43.579	9.147	23.759		0.00	3A4
ATOM	670	C	LEU	132	44.339	12.896	21.142	1.00	0.00	3A4
ATOM	671	0	LEU	132	44.709	12.862	19.975	1.00	0.00	3A4
ATOM	672	N	SER		43.808	14.009	21.685		0.00	3A4 3A4
ATOM ATOM	673 674	CA CB	SER SER		43.570 42.882	15.239 16.277	20.967 21.854		0.00	3A4
ATOM	675	OG	SER		43.525	16.664	23.058		0.00	3A4
ATOM	676	c	SER		44.766	15.878	20.280	1.00	0.00	3A4
ATOM	677	0	SER		44.586	16.429	19.192	1.00	0.00	3A4

ATOM	678	N	PRO	134	46.017	15.798	20.777	1.00	0.00	3A4
MOTA	679	CA	PRO	134	47.159	16.327	20.076	1.00	0.00	3A4 3A4
ATOM	680 681	CD CB	PRO PRO	134 134	46.405 48.327	15.537 16.318	22.155 21.087	1.00	0.00	3A4
ATOM ATOM	682	CG	PRO	134	47.635	16.387	22.434	1.00	0.00	3A4
ATOM	683	C	PRO	134	47.567	15.563	18.844	1.00	0.00	3A4
MOTA	684	0	PRO	134	48.106	16.175	17.927	1.00	0.00	3A4
MOTA	685	N	THR	135	47.305	14.235	18.803	1.00	0.00	3A4
ATOM	686	CA	THR	135	47.657	13.342	17.727 18.232	1.00	0.00	3A4 3A4
ATOM ATOM	687 688	CB OG1	THR THR	135 135	47.864 46.681	11.912 11.299	18.729	1.00	0.00	3A4
ATOM	689		THR	135	48.889	11.953	19.387	1.00	0.00	3A4
ATOM	690	C	THR	135	46.639	13.419	16.594	1.00	0.00	3A4
ATOM	691	0	THR	135	46.921	13.057	15.460	1.00	0.00	3A4
ATOM	692	N	PHE	136	45.420	13.916 13.979	16.895 15.962	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	693 694	CA CB	PHE PHE	136 136	44.322 43.007	13.434	16.581	1.00	0.00	3A4
ATOM	695	CG	PHE	136	43.069	12.028	17.109	1.00	0.00	3A4
ATOM	696		PHE	136	42.397	11.733	18.297	1.00	0.00	3A4
ATOM	697	CD2	PHE	136	43.793	10.992	16.495	1.00	0.00	3A4
ATOM	698		PHE	136	42.237	10.417	18.717	1.00	0.00	3A4
ATOM	699		PHE	136	43.668	9.665 9.372	16.926 18.017	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	700 701	CZ C	PHE	136 136	42.847 44.074	15.402	15.465	1.00	0.00	3A4
ATOM	702	ŏ	PHE	136	42.971	15.703	15.025	1.00	0.00	3A4
ATOM	703	N	THR	137	45.088	16.323	15.493	1.00	0.00	3A4
ATOM	704	CA	THR	137	44.944	17.764	15.224	1.00	0.00	3A4
MOTA	705	CB	THR	137	46.098	18.572	15.830	1.00	0.00	3A4 3A4
ATOM ATOM	706 707	OG1	THR THR	137 137	46.156 45.936	18.321 20.108	17.228 15.640	1.00 1.00	0.00	3A4
ATOM	708	C	THR	137	44.796	18.094	13.739	1.00	0.00	3A4
ATOM	709	Ō	THR	137	43.885	18.830	13.359	1.00	0.00	3A4
ATOM	710	N	SER	138	45.685	17.534	12.870	1.00	0.00	3A4
MOTA	711	CA	SER	138	45.656	17.677	11.419	1.00	0.00	3A4 3A4
ATOM	712	CB OG	SER	138 138	47.076 47.648	17.874 19.086	10.806 11.280	1.00	0.00	3A4
ATOM ATOM	.713 714	C	SER SER	138	45.012	16.431	10.860	1.00	0.00	3A4
ATOM	715	ŏ	SER	138	43.868	16.450	10.408	1.00	0.00	3A4
MOTA	716	N	GLY	139	45.756	15.304	10.953	1.00	0.00	3A4
ATOM	717	CA	GLY	139	45.288	13.957	10.734	1.00	0.00	3A4
ATOM	718	c	GLY	139 139	45.698 46.061	13.207 13.818	11.960 12.961	1.00	0.00	3A4 3A4
ATOM ATOM	719 720	O N	GLY LYS	140	45.629	11.847	11.918	1.00	0.00	3A4
ATOM	721	CA	LYS	140	45.777	10.945	13.054	1.00	0.00	3A4
ATOM	722	CB	LYS	140	44.729	9.786	13.048	1.00	0.00	3A4
ATOM	723	CG	LYS	140	43.246	10.097	13.336	1.00	0.00	3A4
ATOM	724 725	CD CE	LYS LYS	140 140	42.846 41.456	11.560 11.872	13.252 13.770	1.00	0.00	3A4 3A4
ATOM ATOM	726	NZ	LYS	140	41.193	13.331	13.606	1.00	0.00	3A4
ATOM	727	C	LYS	140	47.165	10.340	13.065	1.00	0.00	3A4
ATOM	728	0	LYS	140	47.330	9.123	12.976	1.00	0.00	3A4
ATOM	729	N	LEU	141	48.195	11.212	13.185	1.00	0.00	3A4 3A4
ATOM ATOM	730 731	CA CB	LEU	141 141	49.585 50.096	10.835 10.321	13.207 11.825	1.00	0.00	3A4
ATOM	732	CG	LEU	141	51.411	9.530	11.812	1.00	0.00	3A4
ATOM	733		LEU	141	52.059	9.603	10.425	1.00	0.00	3A4
ATOM	734	CD2	LEU	141	51.161	8.066	12.211	1.00	0.00	3A4
ATOM	735	С	LEU	141	50.286	12.100	13.623	1.00	0.00	3A4
ATOM	736 737	о И	LEU Lys	141 142	50.455 50.687	12.362 12.924	14.813 12.618	1.00	0.00	3A4 3A4
ATOM ATOM	738	CA	LYS	142	51.307	14.222	12.760	1.00	0.00	3A4
ATOM	739	СВ	LYS	142	52.868	14.192	12.729		0.00	3A4
MOTA	740	CG	LYS	142	53.516	13.465	13.915		0.00	3A4
MOTA	741	CD	LYS	142	55.045	13.555	13.916		0.00	3A4
ATOM	742	CE	LYS	142	55.714 55.454	12.858 11.401	15.108 15.086		0.00	3A4 3A4
ATOM ATOM	743 744	NZ C	LYS LYS	142 142	55.454 50.813	15.068	11.606		0.00	3A4
ATOM	745	Ö	LYS	142	50.704	16.287	11.736		0.00	3A4
ATOM	746	N	GLU	143	50.529	14.432	10.433		0.00	3A4
MOTA	747	CA	GLU	143	50.169	15.105	9.198		0.00	3A4
ATOM	748		GLU		51.389	15.242	8.234		0.00	3A4 3A4
ATOM	749	CG	GLU	143	51.158	16.046	6.935	1.00	0.00	JA4

ATOM	750	CD	GLU	143	50.774	17.493	7.267		0.00	3A4
ATOM	751	OE1		143		18.194	7.909		0.00 0.00	3A4 3A4
ATOM	752	OE2		143		17.917	6.882 8.559	1.00	0.00	3A4
ATOM	753	С 0	GLU GLU	143 143	49.047 47.898	14.324 14.760	8.605	1.00	0.00	3A4
ATOM ATOM	754 755	N	MET	144	49.393	13.160	7.926	1.00	0.00	3A4
ATOM	756	CA	MET	144	48.584	12.130	7.300	1.00	0.00	3A4
ATOM	757	СВ	MET	144	47.303	11.759	8.070	1.00	0.00	3A4
MOTA	758	CG	MET	144	47.567	10.932	9.334	1.00	0.00	3A4
MOTA	759	SD	MET	144	48.269	9.267	9.019	1.00	0.00	3A4 3A4
ATOM	760	CE	MET MET	144 144	47.029 48.192	8.504 12.409	7.928 5.879	1.00	0.00	3A4
ATOM ATOM	761 762	0	MET	144	47.891	11.472	5.150	1.00	0.00	3A4
ATOM	763	N	VAL	145	48.169	13.678	5.428	1.00	0.00	3A4
MOTA	764	CA	VAL	145	47.650	14.088	4.130	1.00	0.00	3A4
ATOM	765	СB	VAL	145	47.693	15.597	3.949	1.00	0.00	3A4 3A4
ATOM	766		VAL	145	46.839	16.061	2.734 5.237	1.00	0.00	3A4
ATOM	76 7 768		VAL	145 145	47.128 48.261	16.245 13.425	2.906	1.00	0.00	3A4
ATOM ATOM	769	C O	VAL VAL	145	47.501	13.014	2.026	1.00	0.00	3A4
ATOM	770	N	PRO	146	49.595	13.235	2.821	1.00	0.00	3A4
ATOM	771	CA	PRO	146	50.226	12.490	1.741	1.00	0.00	3A4
MOTA	772	CD	PRO	146	50.623	13.942	3.599	1.00	0.00	3A4
MOTA	773	CB	PRO	146	51.743	12.625	1.988	1.00	0.00 0.00	3A4 3A4
ATOM	774	CG	PRO	146	51.872 49.826	13.954 11.029	2.721 1.698	1.00	0.00	3A4
MOTA MOTA	775 776	C O	PRO PRO	146 146	49.678	10.483	0.613	1.00	0.00	3A4
ATOM	777	N	ILE	147	49.572	10.388	2.863	1.00	0.00	3A4
ATOM	778	CA	ILE	147	49.098	9.027	2.976	1.00	0.00	3A4
MOTA	779	СВ	ILE	147	49.254	8.469	4.382	1.00	0.00	3A4
ATOM	780		ILE	147	48.993	6.930	4.422	1.00	0.00 0.00	3A4 3A4
ATOM	781 782	CG1	ILE	147 147	50.685 51.018	8.809 8.281	4.901 6.300	1.00	0.00	3A4
ATOM ATOM	783	C	ILE	147	47.660	8.881	2.564	1.00	0.00	3A4
ATOM	784	ŏ	ILE	147	47.306	7.899	1.922	1.00	0.00	3A4
ATOM	785	N	ILE	148	46.789	9.866	2.875	1.00	0.00	3A4
MOTA	786	CA	ILE	148	45.386	9.833	2.503	1.00	0.00	3A4
ATOM	787	СВ	ILE	148	44.570	10.932	3.172 2.811	1.00	0.00 0.00	3A4. 3A4
MOTA	788 789	CG2 CG1		148 148	43.057 44.675	10.768 10.809	4.718	1.00	0.00	3A4
ATOM ATOM	790	CD	ILE	148	44.158	12.030	5.488	1.00	0.00	3A4
ATOM	791	c	ILE	148	45.218	9.888	1.005	1.00	0.00	3A4
MOTA	792	0	ILE	148	44.486	9.106	0.407	1.00	0.00	3A4
ATOM	793	N	ALA	149	46.000	10.765	0.350	1.00	0.00	3A4 3A4
ATOM	794	CA	ALA	149	46.058 46.983	10.923 12.097	-1.086 -1.414	1.00	0.00	3A4
ATOM ATOM	795 796	CB C	ALA ALA	149 149	46.539	9.682	-1.803	1.00	0.00	3A4
ATOM	797	ō	ALA	149	45.965	9.246	-2.797	1.00	0.00	3A4
ATOM	798	N	GLN	150	47.578	9.019	-1.243	1.00	0.00	3A4
MOTA	799	ÇA	GLN	150	48.121	7.780	-1.753	1.00	0.00	3A4
MOTA	800	CB	GLN	150	49.342	7.295	-0.954	1.00	0.00 0.00	3A4 3A4
ATOM	801 802	CD	GLN GLN	150 150	50.637 51.737	8.037 7.586	-1.297 -0.326	1.00	0.00	3A4
ATOM ATOM	803	OE1		150	52.080	6.406	-0.292	1.00		3A4
ATOM	804	NE2		150	52.300	8.525	0.483	1.00	0.00	3A4
MOTA	805	С	GLN	150	47.129	6.663	-1.774	1.00		3A4
MOTA	806	0	GLN	150	46.962	5.992	-2.789	1.00		3A4 3A4
MOTA	807	N	TYR	151	46.371	6.500 5.431	-0.658 -0.538	1.00		3A4
ATOM ATOM	808 809	CA CB	TYR TYR	151 151	45.418 44.853	5.227	0.859			3A4
ATOM	810	CG	TYR	151	44.181	3.823	0.880			3A4
MOTA	811		LTYR	151	43.188	3.417	1.745			3A4
ATOM	812	CD2	YYR	151	44.795	2.750	0.124			3A4
ATOM	813		TYR	151	42.443	2.274	1.345			3A4 3A4
ATOM	814	CE2		151	44.170	1.533	-0.113 0.454			3A4 3A4
ATOM ATOM	815 816		TYR TYR	151 151	42.935 42.254	0.104	0.201			3A4
MOTA	817		TYR		44.221	5.669	-1.449			3A4
ATOM	818		TYR		43.738	4.750	-2.103	1.00		3A4
ATOM	819	N	GLY	152	43.775	6.936	-1.554			3A4
ATOM	820		GLY		42.703		-2.423			3A4 3A4
MOTA	821	С	GLY	152	42.962	7.025	-3.877	1.00	0.00	SA4

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ATOM	822	0	GLY	152	42.122	6.466	-4.565	1.00	0.00	3A4
MOTA	823		ASP	153	44.194	7.284	-4.339	1.00	0.00	3A4
ATOM	824	CA	ASP	153	44.647	6.996	-5.674	1.00	0.00	3A4 3A4
MOTA	825	CB	ASP	153	46.061	7.586	-5.844	1.00 1.00	0.00	3A4
MOTA	826 827	CG OD1	ASP	153 153	45.993 45.014	9.119 9.650	-5.945 -6.534	1.00	0.00	3A4
ATOM ATOM	828	OD2		153	46.922	9.784	-5.416	1.00	0.00	3A4
ATOM	829	C	ASP	153	44.703	5.521	-6.007	1.00	0.00	3A4
MOTA	830	ō	ASP	153	44.288	5.096	-7.076	1.00	0.00	3A4
ATOM	831	N	VAL	154	45.154	4.686	-5.048	1.00	0.00	3A4
ATOM	832	CA	VAL	154	45.173	3.235	-5.160	1.00	0.00	3A4
MOTA	833	CB	VAL	154	45.878	2.605	-3.968	1.00	0.00	3A4
ATOM	834	CG1		154	45.770	1.054	-3.875	1.00	0.00	3A4
ATOM	835	CG2		154	47.373	2.989	-4.067	1.00	0.00	3A4
ATOM	836	Ç	VAL	154	43.793	2.651	-5.283	1.00	0.00	3A4 3A4
MOTA	837	0	VAL	154 155	43.531 42.842	1.783	-6.112 -4.494	1.00 1.00	0.00	3A4
ATOM ATOM	838 839	N CA	LEU	155	41.460	2.758	-4.505	1.00	0.00	3A4
ATOM	840	CB	LEU	155	40.697	3.480	-3.395	1.00	0.00	3A4
ATOM	841	CG	LEU	155	41.005	3.018	-1.989	1.00	0.00	3A4
ATOM	842	CD1		155	40.785	4.226	-1.096	1.00	0.00	3A4
MOTA	843	CD2	LEU	155	40.117	1.825	-1.591	1.00	0.00	3A4
ATOM	844	С	LEU	155	40.732	3.082	-5.782	1.00	0.00	3A4
MOTA	845	0	LEU	155	39.955	2.295	-6.313	1.00	0.00	3A4
ATOM	846	N	VAL	156	41.020	4.276	-6.333	1.00	0.00	3A4
ATOM	847	CA	VAL	156	40.441	4.744	-7.564	1.00	0.00	3A4
ATOM	848	CB	VAL	156	40.709	6.216	-7.769	1.00	0.00 0.00	3A4 3A4
ATOM	849		VAL	156	40.208 39.887	6.709 6.989	-9.147 -6.709	1.00 1.00	0.00	3A4
ATOM ATOM	850 851	CGZ	VAL VAL	156 156	40.956	3.916	-8.726	1.00	0.00	3A4
ATOM	852	0	VAL	156	40.186	3.474	-9.566	1.00	0.00	3A4
ATOM	853	N ·	ARG	157	42.263	3.571	-8.714	1.00	0.00	3A4
ATOM	854	CA	ARG	157	42.881	2.692	-9.687	1.00	0.00	3A4
ATOM	855	СВ	ARG	157	44.400	2.603	-9.480	1.00	0.00	3A4
ATOM	856	CG	ARG	157	45.201		-10.646	1.00	0.00	3A4
MOTA	857	CD	ARG	157	46.718	•	-10.406	1.00	0.00	3A4
ATOM	858	NE	ARG	157	47.008	0.982	-9.282	1.00	0.00	3A4
ATOM	859	CZ	ARG	157	47.582	1.328	-8.084	1.00	0.00	3A4 3A4
ATOM	860		ARG	157 157	47.753 47.975	0.362 2.607	-7.136 -7.807	1.00	0.00	3A4
ATOM ATOM	861 862	C	ARG ARG	157	42.316	1.305	-9.694	1.00	0.00	3A4
ATOM	863	Ö	ARG	157	42.062		-10.749	1.00	0.00	3A4
ATOM	864	N	ASN	158	42.004	0.746	-8.509	1.00	0.00	3A4
ATOM	865	CA	ASN	158	41.363	-0.540	-8.359	1.00	0.00	3A4
ATOM	866	СВ	ASN	158	41.312	-0.962	-6.875	1.00	0.00	3A4
MOTA	867	CG	ASN	158	42.725	-1.184	-6.308	1.00	0.00	3A4
MOTA	868		ASN	158	43.710	-1.336	-7.029	1.00	0.00	3A4
ATOM	869		ASN	158	42.827	-1.211	-4.951	1.00	0.00	3A4 3A4
ATOM	870	C	ASN	158	39.959 39.541	-0.569 -1.568	-8.928 -9.503	1.00	0.00	3A4
ATOM ATOM	871 872	О И	ASN LEU	158 159	39.205	0.547	-8.840	1.00	0.00	3A4
ATOM	873	CA	LEU	159	37.900	0.698	-9.460	1.00	0.00	3A4
ATOM	874	СB	LEU	159	37.181	1.944		1.00	0.00	3A4
ATOM	875	CG	LEU	159	36.392	1.845			0.00	3A4
ATOM	876		LEU	159	35.846	3.252	-7.275	1.00	0.00	3A4
MOTA	877	CD2	LEU	159	35.226	0.844			0.00	3A4
MOTA	878	С	LEU	159	37.986		-10.979		0.00	3A4
ATOM	879	0	LEU	159	37.180		-11.731		0.00	3A4
ATOM	880	N	ARG	160	39.032		-11.475		0.00	3A4 3A4
ATOM	881	CA	ARG	160	39.316 40.462		-12.887 -13.097		0.00	3A4
ATOM	882 883	CB CG	ARG	160 160	40.462		-12.829		0.00	3A4
ATOM ATOM	884	CD	ARG ARG	160	41.097		-13.106		0.00	3A4
ATOM	885	NE	ARG	160	42.243		-12.147		0.00	3A4
ATOM	886	CZ	ARG	160	43.077		-11.785		0.00	3A4
ATOM	887		ARG	160	44.114		-10.932	1.00		3A4
ATOM	888	NH2	ARG	160	42.889		-12.251			3A4
ATOM	889	C	ARG	160	39.687		-13.585			3A4
MOTA	890	0	ARG	160	39.428		-14.767			3A4
ATOM	891	N	ARG	161	40.250		-12.834			3A4 3A4
MOTA	892	CA	ARG	161 161	40.597 41.743) -13.293 ! -12.420			3A4 3A4
ATOM	893	СВ	ARG	161	41.743	-4.432	16.420		5.00	JAT

ATOM	894	CG	ARG	161		-1.717 -			0.00	3A4
ATOM	895	CD	ARG	161		-1.838 -			0.00	3A4 3A4
ATOM	896	NE CZ	ARG ARG	161 161	44.400 45.172	-3.285 - -3.692 -		1.00	0.00	3A4
ATOM ATOM	897 898	NH1		161	45.396	-5.024 -		1.00	0.00	3A4
ATOM	899	NH2		161	45.720	-2.792	-9.328	1.00	0.00	3A4
ATOM	900	С	ARG	161	39.432	-2.837 -	-13.270	1.00	0.00	3A4
MOTA	901	0	ARG	161	39.618	-4.026 ·		1.00	0.00	3A4
ATOM	902	N	GLU	162	38.181	-2.341		1.00	0.00	3A4
ATOM	903	CA	GLU	162	36.943 35.704	-3.106 · -2.403 ·		1.00	0.00	3A4 3A4
ATOM ATOM	904 905	CB CG	GLU	162 162	35.006	-1.245		1.00	0.00	3A4
ATOM	906	CD	GLU	162	33.961	-0.524		1.00	0.00	3A4
ATOM	907	OE1		162	34.331	-0.002	-11.289	1.00	0.00	3A4
ATOM	908	OE2		162	32.779	-0.469		1.00	0.00	3A4
ATOM	909	С	GLU	162	36.578	-3.419		1.00	0.00	3A4 3A4
ATOM	910	0	GLU	162 163	36.521 36.386	-2.577 -4.746		1.00	0.00	3A4
ATOM ATOM	911 912	N CA	ALA ALA	163	36.408	-5.391		1.00	0.00	3A4
ATOM	913	СВ	ALA	163	37.029	-6.809		1.00	0.00	3A4
ATOM	914	С	ALA	163	35.037	-5.494		1.00	0.00	3A4
MOTA	915	0	ALA	163	34.019	-5.308		1.00	0.00	3A4
ATOM	916	N	GLU	164	35.042		-18.059	1.00	0.00	3A4 3A4
ATOM	917 918	CA CB	GLU	164 164	33.935 32.661		-19.009 -18.459	1.00	0.00	3A4
ATOM ATOM	919	CG	GLU	164	31.701		-19.531	1.00	0.00	3A4
ATOM	920	CD	GLU	164	30.505		-18.839	1.00	0.00	3A4
ATOM	921		GLU	164	29.737		-18.156	1.00	0.00	3A4
ATOM	922		GLU	164	30.342		-18.984	1.00	0.00	3A4
ATOM	923	C	GLU	164	33.612		-19.520	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	924 925	O N	GLU THR	164 165	32.462 34.671		-19.797 -19.572	1.00	0.00	3A4
ATOM	926	CA	THR	165	34.730		-19.714	1.00	0.00	3A4
ATOM	927	СВ	THR	165	34.039	-1.480	-20.938	1.00	0.00	3A4
MOTA	928	OG1	THR	165	32.615		-20.965	1.00	0.00	3A4
ATOM	929		THR	165	34.604		-22.228	1.00	0.00	3A4 3A4
ATOM	930	C	THR	165	34.372 35.235		-18.379 -17.690	1.00	0.00 0.00	3A4
ATOM ATOM	931 932	O N	THR GLY	165 166	33.233		-17.996	1.00	0.00	3A4
ATOM	933	CA	GLY	166	32.567		-16.720	1.00	0.00	3A4
ATOM	934	С	GLY	166	31.084	-1.094	-16.877	1.00	0.00	3A4
ATOM	935	0	GLY	166	30.541		-17.449	1.00	0.00	3A4
ATOM	936	N	LYS	167	30.386		-16.363 -16.262	1.00	0.00	3A4 3A4
ATOM ATOM	937 938	CA CB	LYS LYS	167 167	28.935 28.217		-17.239	1.00	0.00	3A4
ATOM	939	CG	LYS	167	28.165		-18.713	1.00	0.00	3A4
ATOM	940	CD	LYS	167	29.336	-3.252	-19.574	1.00	0.00	3A4
ATOM	941	CE	LYS	167	29.134		-21.066	1.00	0.00	3A4
MOTA	942	NZ	ĻYS	167	30.208		-21.890	1.00	0.00	3A4 3A4
ATOM ATOM	943 944	С 0	LYS LYS	167 167	28.582 27.816		-14.802 -14.271	1.00	0.00	3A4
ATOM	945	N	PRO	168	29.041		-14.057	1.00	0.00	3A4
ATOM	946	CA	PRO	168	28.796		-12.622	1.00	0.00	3A4
MOTA	947	CD	PRO	168	29.518		-14.626	1.00	0.00	3A4
MOTA	948	СВ	PRO	168	28.695		-12.400	1.00	0.00	3A4 3A4
ATOM	949	CG	PRO		29.625 29.938		-13.459 -11.812	1.00	0.00	3A4 3A4
ATOM ATOM	950 951	С 0	PRO PRO		31.100		-12.110	1.00	0.00	3A4
ATOM	952	N	VAL	169	29.609		-10.724	1.00	0.00	3A4
ATOM	953	CA	VAL	169	30.441	-2.280		1.00	0.00	3A4
ATOM	954	СВ	VAL	169	31.674	-1.381	-9.591	1.00	0.00	3A4
MOTA	955		VAL		31.356	0.130			0.00	3A4 3A4
ATOM	956 957		VAL		32.702 29.535	-1.746 -1.926				3A4
ATOM ATOM	95 <i>1</i> 958	С 0	VAL VAL		28.623	-1.120				3A4
ATOM	959	Ŋ	THR		29.805	-2.498	-7.184	1.00	0.00	3A4
ATOM	960	CA	THR	170	29.193	-2.121				3A4
ATOM	961	СВ	THR		28.902	-3.314				3A4
ATOM	962		THR		28.066 28.173	-4.231 -2.877				3A4 3A4
ATOM ATOM	963 964	CGZ	THR THR		30.178	-1.183				3A4
MOTA	965	ŏ	THR		31.232	-1.589				3A4

ATOM	966	N	LEU	171	29.854	0.126	-5.296	1.00	0.00	3A4
ATOM	967	CA	LEU	171	30.705	1.177	-4.769	1.00	0.00	3A4
MOTA	968	СB	LEU	171	30.055	2.555	-5.044	1.00	0.00	3A4
MOTA	969	CG	LEU	171	30.547	3.319	-6.282	1.00	0.00	3A4
MOTA	970	CD1		171	29.654	4.563	-6.453	1.00	0.00	3A4
ATOM	971	CD2		171	32.040	3.710	-6.194	1.00	0.00	3A4 3A4
MOTA	972	C	LEU	171	30.998	1.069	-3.277	1.00	0.00	3A4
MOTA	973	0	LEU	171	32.076	1.436	-2.831 -2.464	1.00	0.00	3A4
ATOM	974	N	LYS	172	30.072 30.261	0.510 0.291	-1.041	1.00	0.00	3A4
ATOM	975	CA CB	LYS LYS	172 172	28.920	-0.132	-0.376	1.00	0.00	3A4
ATOM ATOM	976 977	CG	LYS	172	28.909	-0.334	1.158	1.00	0.00	3A4
ATOM	978	CD	LYS	172	29.194	0.939	1.969	1.00	0.00	3A4
ATOM	979	CE	LYS	172	29.078	0.766	3.488	1.00	0.00	3A4
ATOM	980	NZ	LYS	172	30.110	-0.160	4.012	1.00	0.00	3A4
ATOM	981	С	LYS	172	31.330	-0.744	-0.748	1.00	0.00	3A4
MOTA	982	0	LYS	172	32.274	-0.492	-0.010	1.00	0.00	3A4
ATOM	983	N	ASP	173	31.243	-1.937	-1.374	1.00	0.00	3A4
MOTA	984	CA	ASP	173	32.134	-3.048	-1.103	1.00	0.00	3A4
ATOM	985	CB	ASP	173	31.447	-4.365	-1.539	1.00	0.00	3A4 3A4
MOTA	986	CG	ASP	173	32.095	-5.634	-0.940	1.00	0.00 0.00	3A4
MOTA	987		ASP	173	32.129 32.559	-5.750 -6.496	0.315 -1.735	1.00	0.00	3A4
ATOM	988		ASP	173 173	33.491	-2.909	-1.760	1.00	0.00	3A4
ATOM	989 990	с 0	ASP ASP	173	34.487	-3.361	-1.199	1.00	0.00	3A4
ATOM ATOM	991	Ŋ	VAL	174	33.571	-2.272	-2.947	1.00	0.00	3A4
ATOM	992	CA	VAL	174	34.804	-2.128	-3.702	1.00	0.00	3A4
ATOM	993	СВ	VAL	174	34.550	-2.192	-5.209	1.00	0.00	3A4
ATOM	994		VAL	174	35.866	-2.225	-6.033	1.00	0.00	3A4
ATOM	995	CG2	VAL	174	33.783	-3.513	-5.482	1.00	0.00	3A4
MOTA	996	С	VAL	174	35.560	-0.866	-3.321	1.00	0.00	3A4
MOTA	997	0	VAL	174	36.767	-0.793	-3.522	1.00	0.00	3A4 3A4
ATOM	998	N	PHE	175	34.889	0.162	-2.748	1.00	0.00 0.00	3A4 3A4
ATOM	999	CA	PHE	175	35.513	1.457	-2.585	1.00	0.00	3A4
ATOM	1000	CB	PHE	175	34.996 35.738	2.458 3.789	-3.637 -3.669	1.00	0.00	3A4
MOTA	1001	CG	PHE	175 175	35.169	4.936	-3.079	1.00	0.00	3A4
ATOM ATOM	1002 1003		PHE	175	37.019	3.896	-4.239	1.00	0.00	3A4
ATOM	1003		PHE	175	35.866	6.153	-3.047	1.00	0.00	3A4
ATOM	1005		PHE	175	37.703	5.120	-4.237	1.00	0.00	3A4
ATOM	1006	CZ	PHE	175	37.136	6.244	-3.628	1.00	0.00	3A4
ATOM	1007	С	PHE	175	35.362	1.997	-1.219	1.00	0.00	3A4
ATOM	1008	0	PHE	175	36.347	2.184	-0.509	1.00	0.00	3A4
MOTA	1009	N	GLY	176	34.105	2.318	-0.836	1.00	0.00	3A4
MOTA	1010	CA	GLY	176	33.755	3.060	0.352	1.00	0.00	3A4 3A4
MOTA	1011	С	GLY	176	34.098	2.332	1.609	1.00	0.00	3A4
ATOM	1012	0	GLY	176	34.413	2.958 0.976	2.614 1.565	1.00	0.00	3A4
ATOM	1013	N	ALA	177 1 77	34.126 34.485	0.376	2.688	1.00	0.00	3A4
ATOM ATOM	1014 1015	CA CB	ALA ALA	177	33.968	-1.294	2.532	1.00	0.00	3A4
ATOM	1015	C	ALA	177	35.962	0.124	2.957	1.00	0.00	3A4
ATOM	1017	ŏ	ALA	177	36.406	0.327	4.080	1.00	0.00	3A4
ATOM	1018	N	TYR	178	36.777	-0.058	1.903	1.00	0.00	3A4
ATOM	1019	CA	TYR	178	38.203	-0.242	2.016			3A4
ATOM	1020	СВ	TYR	178	38.721	-0.724	0.638			3A4
ATOM	1021	CG	TYR	178	38.656	-2.235	0.593			3A4
ATOM	1022		LTYR	178	37.893	-2.854	-0.416			3A4
ATOM	1023		YYR	178	39.236	-3.052	1.584			3A4 3A4
ATOM	1024		LTYR	178	37.711	-4.243				3A4
ATOM	1025		TYR	178	39.039 38.282	-4.442 -5.040				3A4
ATOM	1026	CŻ	TYR	178 178	38.091	-6.439				3A4
ATOM ATOM	1027 1028	OH C	TYR TYR	178	38.966	1.017				3A4
ATOM	1028	0	TYR		39.918	0.985				3A4
ATOM	1030	N	SER		38.545	2.180				3A4
ATOM	1031	CA	SER		39.171	3.471				3A4
ATOM	1032	CB	SER		38.412	4.545	1.196	1.00		3A4
ATOM	1033		SER		39.108	5.787				3A4
MOTA	1034	¢	SER		39.344	3.878				3A4
MOTA	1035		SER		40.445	4.039				3A4
MOTA	1036		MET		38.263					3A4 3A4
ATOM	1037	CA	MET	180	38.328	4.314	5.62	1.00	0.00	JA4

MOTA	1038	СВ	MET	180	36.898	4.623	5.984	1.00	0.00	3A4
MOTA	1039	CG	MET	180	36.729	5.941	5.189	1.00	0.00	3A4
ATOM	1040	SD	MET	180	35.589	5.903	3.791	1.00	0.00	3A4 3A4
MOTA	1041 1042	CE	MET MET	180 180	36.564 38.961	7.153 3.325	2.893 6.527	1.00	0.00	3A4
MOTA MOTA	1042	0	MET	180	39.602	3.684	7.513	1.00	0.00	3A4
ATOM	1044	N	ASP	181	38.892	2.030	6.144	1.00	0.00	3A4
ATOM	1045	CA	ASP	181	39.455	1.016	6.971	1.00	0.00	3A4
MOTA	1046	СВ	ASP	181	38.927	-0.386	6.705	1.00	0.00	3A4
ATOM	1047	CG	ASP	181	38.781	-1.148	5.400	1.00	0.00	3A4
ATOM	1048	OD1 OD2		181 181	39.773 37.728	-1.165 -1.810	4.635 5.195	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1049 1050	C	ASP	181	40.963	0.976	6.884	1.00	0.00	3A4
ATOM	1051	ŏ	ASP	181	41.663	0.876	7.886	1.00	0.00	3A4
ATOM	1052	N	VAL	182	41.515	1.163	5.671	1.00	0.00	3A4
ATOM	1053	CA	VAL	182	42.946	1.238	5.464	1.00	0.00	3A4
ATOM	1054	СВ	VAL	182	43.279	1.227	4.010	1.00	0.00	3A4 3A4
ATOM ATOM	1055 1056		VAL VAL	182 182	44.767 42.889	1.508 -0.181	3.706 3.532	1.00 1.00	0.00 0.00	3A4 3A4
MOTA	1057	C	VAL	182	43.593	2.408	6.151	1.00	0.00	3A4
ATOM	1058	ŏ	VAL	182	44.676	2.298	6.708	1.00	0.00	3A4
ATOM	1059	N	ILE	183	42.877	3.540	6.210	1.00	0.00	3A4
MOTA	1060	CA	ILE	183	43.341	4.740	6.855	1.00	0.00	3A4
MOTA	1061	CB	ILE	183	42.480	5.913	6.432	1.00	0.00	3A4
ATOM	1062		ILE	183 183	42.783 42.712	7.205 6.215	7.220 4.926	1.00	0.00	3A4 3A4
ATOM ATOM	1063 1064	CD	ILE	183	44.121	6.672	4.516	1.00	0.00	3A4
ATOM	1065	c	ILE	183	43.365	4.589	8.352	1.00	0.00	3A4
MOTA	1066	0	ILE	183	44.321	4.972	9.017	1.00	0.00	3A4
MOTA	1067	N	THR	184	42.323	3.969	8.947	1.00	0.00	3A4
MOTA	1068	CA	THR	184	42.311	3.780	10.379	1.00	0.00	3A4 3A4
MOTA MOTA	1069 1070	CB	THR THR	184 184	40.896 40.842	3.599 3.873	10.968 12.369	1.00	0.00 0.00	3A4
ATOM	1070		THR	184	40.253	2.222	10.686	1.00	0.00	3A4
ATOM	1072	c	THR	184	43.288	2.710	10.811	1.00	0.00	3A4
ATOM	1073	0	THR	184	43.934	2.838	11.842	1.00	0.00	3A4
ATOM	1074	N	SER	185	43.544	1.697	9.955	1.00	0.00	3A4
ATOM	1075	CA	SER	185	44.571	0.701	10.179	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1076 1077	CB OG	SER SER	185 185	44.486 43.278	-0.452 -1.178	9.173 9.354	1.00	0.00	3A4
ATOM	1078	ç	SER	185	45.975	1.270	10.157	1.00	0.00	3A4
ATOM	1079	0	SER	185	46.793	0.962	11.011	1.00	0.00	3A4
MOTA	1080	N	THR	186	46.255	2.211	9.238	1.00	0.00	3A4
ATOM	1081	CA	THR	186	47.523	2.905	9.158	1.00	0.00	3A4 3A4
ATOM	1082 1083	CB OG1	THR THR	186 186	47.67 4 46.613	3.626 4.495	7.845 7.478	1.00	0.00	3A4
ATOM ATOM	1084	CG2		186	47.869	2.559	6.746	1.00	0.00	3A4
ATOM	1085	c	THR	186	47.770	3.895	10.256	1.00	0.00	3A4
MOTA	1086	0	THR	186	48.906	4.171	10.627	1.00	0.00	3A4
ATOM	1087	N	SER	187	46.676	4.433	10.825	1.00	0.00	3A4
MOTA MOTA	1088 1089	CA CB	SER	187 187	46.674 45.260	5.311 5.983	11.961 12.078	1.00	0.00	3A4 3A4
ATOM	1099		SER	187	45.037	6.742	13.262	1.00	0.00	3A4
ATOM	1091	c	SER	187	47.012	4.556	13.221	1.00	0.00	3A4
MOTA	1092	0	SER	187	47.753	5.052	14.047	1.00	0.00	3A4
ATOM	1093		PHE	188	46.490	3.324	13.352	1.00	0.00	3A4
ATOM	1094	CA	PHE	188	46.634	2.477	14.511	1.00	0.00	3A4 3A4
ATOM ATOM	1095 1096	CB CG	PHE	188 188	45.408 44.440	1.520 2.221	14.609 15.507	1.00	0.00	3A4
ATOM	1097		PHE	188	43.828	3.428	15.112		0.00	3A4
ATOM	1098		PHE	188	44.425	1.853	16.860		0.00	3A4
ATOM	1099		PHE	188	43.309	4.298	16.068		0.00	3A4
ATOM	1100		PHE	188	43.917	2.727	17.815		0.00	3A4
ATOM	1101		PHE	188	43.370 47.882	3.945 1.665	17.418 14.537		0.00	3A4 3A4
ATOM ATOM	1102 1103		PHE PHE	188 188	48.386	1.332	15.605		0.00	3A4
ATOM	1104		GLY		48.414	1.335	13.350			3A4
ATOM	1105		GLY	189	49.610	0.550	13.208	1.00		3A4
MOTA	1106		GLY		49.281	-0.923	13.101			3A4
ATOM	1107		GLY		50.025	-1.788	13.555			3A4 3A4
MOTA MOTA	1108 1109		VAL VAL		48.147 47.745	-1.240 -2.576	12.428 12.011			3A4
W + Ot 1	1103	~~	* 1714	100						

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3A4 MOTA 1110 CB VAL 190 46.239 -2.768 11.929 1.00 0.00 45.823 -4.253 11.759 1.00 0.00 3A4 CG1 VAL 190 MOTA 1111 1.00 0.00 3A4 VAI. 45.621 -2.21713.235 ATOM 1112 CG2 190 1.00 3A4 0.00 ATOM 1113 С VAL 190 48.306 -2.84310.635 MOTA 1114 0 VAL 190 48.419 -1.948 9.801 1.00 0.00 3A4 -4.105 1.00 0.00 3A4 48.675 10.372 1115 ASN 191 ATOM N -4.477 9.377 1.00 0.00 3A4 49.636 ASN 191 ATOM 1116 CA 1.00 0.00 3A4 9.517 ATOM 1117 CB ASN 191 49.869 -5.997 1.00 191 51.211 -6.5028.934 0.00 3A4 MOTA 1118 CG ASN 52.277 -6.160 9.445 1.00 0.00 3A4 MOTA 1119 OD1 ASN 191 1.00 0.00 3A4 51.156 -7.322 7.848 191 ATOM 1120 ND2 ASN 1.00 0.00 3A4 MOTA 1121 C ASN 191 49.394 -4.146 7.970 1122 1.00 0.00 3A4 0 ASN 191 48.268 -4.3637.523 ATOM 192 50.505 -3.532 7.398 1.00 0.00 3A4 ATOM 1123 N ILE 1.00 0.00 3A4 192 50.796 -3.011 6.064 ATOM 1124 CA ILE 49.572 -3.045 5.191 1.00 0.00 3A4 192 ATOM 1125 CB ILE 5.843 1.00 0.00 3A4 -2.012 1126 CG2 ILE 192 48.539 MOTA 0.00 3A4 CG1 ILE 192 49.850 -3.205 3.643 1.00 ATOM 1127 50.855 -4.296 3.249 1.00 0.00 3A4 ATOM 1128 CD ILE 192 3A4 51.332 -1.562 6.101 1.00 0.00 ILE 192 ATOM 1129 C. 0.00 3A4 1.00 ATOM 1130 0 TLE 192 51.714 -1.0497.152 1.00 3A4 0.00 ASP 193 51.273 -0.876 4.912 ATOM 1131 N 51.280 ATOM 1132 CA ASP 193 0.551 4.649 1.00 0.00 3A4 193 52.500 0.950 3.755 1.00 0.00 3A4 ASP 1133 CB ATOM 2.473 3.713 1.00 0.00 3A4 52.747 ATOM 1134 CG ASP 193 3A4 1.00 0.00 3.055 2.596 ATOM 1135 OD1 ASP 193 52.690 3A4 ATOM 1136 OD2 ASP 193 52.993 3.065 4.798 1.00 0.00 0.941 3.982 1.00 0.00 3A4 1137 ASP 193 49.942 ATOM С 0.00 3A4 49.555 2.107 4.042 1.00 193 1138 o ASP ATOM 1.00 0.00 3A4 3.351 ATOM 1139 N SER 194 49.199 -0.0253A4 0.00 ATOM 1140 CA SER 194 47.801 0.108 2.935 1.00 194 47.674 0.859 1.564 1.00 0.00 3A4 ATOM 1141 CB SER 0.364 0.570 1.00 0.00 3A4 OG SER 194 48.568 1142 ATOM 3A4 47.072 -1.263 2.877 1.00 0.00 ATOM 1143 С SER 194 47.201 0.00 3A4 -1.949 1.864 1.00 ATOM 1144 0 SER 194 0.00 3A4 1145 N LEU 195 46.300 -1.6823.968 1.00 ATOM 45.506 -2.928 4.205 1.00 0.00 3A4 ATOM 1146 CA LEU 195 LEU 195 44.616 -3.155 2.908 1.00 0.00 3A4 ATOM 1147 CB 195 43.358 -4.046 2.893 1.00 0.00 3A4 1148 LEU MOTA CG -3.731 1.00 0.00 3A4 42.566 1.614 ATOM 1149 CD1 LEU 195 3A4 0.00 ATOM 1150 CD2 LEU 195 43.591 -5.569 2.963 1.00 46.313 -4.231 4.384 1.00 0.00 3A4 ATOM 1151 C LEU 195 0 LEU 195 46.823 -4.525 3.303 1.00 0.00 3A4 ATOM 1152 -5.133 5.522 1.00 0.00 3A4 196 46.462 1153 ASN ATOM N 3A4 46.660 5.007 1.00 0.00 ATOM 1154 CA ASN 196 -6.447 3A4 ATOM 1155 CB ASN 196 48.141 -6.561 4.645 1.00 0.00 ATOM 1156 CG ASN 196 48.532 -7.677 3.641 1.00 0.00 3A4 1.00 0.00 3A4 OD1 ASN 196 49.287 -8.581 3.992 1157 ATOM 48.039 -7.601 2.374 1.00 0.00 3A4 1158 ND2 ASN 196 ATOM 3A4 46.000 5.603 0.00 ATOM 1159 C ASN 196 -7.578 1.00 ASN 196 44.826 -7.879 5.338 1.00 0.00 3A4 ATOM 1160 0 46.757 -8.297 6.407 1.00 0.00 3A4 1161 ASN 197 ATOM N 3A4 197 46.317 -9.599 6.859 1.00 0.00 CA ASN ATOM 1162 47.456 -10.511 1.00 0.00 3A4 197 7.443 ATOM 1163 CB ASN 3A4 6.405 1.00 0.00 ATOM 1164 CG ASN 197 48.572 -10.689 3A4 197 48.334 -11.249 5.336 1.00 0.00 ATOM 1165 OD1 ASN 49.810 -10.219 6.717 1.00 0.00 3A4 1166 ND2 ASN 197 ATOM 3A4 ATOM 1167 ASN 197 45.160 -9.556 7.804 1.00 0.00 C 44.307 -10.439 7.761 1.00 0.00 3A4 197 **ATOM** 1168 0 ASN 3A4 0.00 MOTA 1169 N PRO 198 45.075 -8.496 8.595 1.00 198 44.013 -8.420 9.555 1.00 0.00 3A4 ATOM 1170 CA PRO MOTA 1171 CD PRO 198 46.277 -7.818 9.154 1.00 0.00 3A4 44.652 -7.631 10.641 1.00 0.00 3A4 198 CB PRO ATOM 1172 46.123 -7.908 10.628 1.00 0.00 3A4 ATOM 1173 CG PRO 198 9.085 0.00 3A4 -7.786 1.00 ATOM 1174 С PRO 198 42.754 ATOM 1175 0 PRO 198 41.799 -7.743 9.865 1.00 0.00 3A4 42.701 -7.279 7.830 1.00 0.00 3A4 1176 199 MOTA GLN N 0.00 3A4 41.636 -6.407 7.407 1.00 1177 GLN 199 ATOM CA 6.066 1.00 0.00 3A4 -5.668 ATOM 1178 CB GLN 199 41.900 5.844 1.00 0.00 3A4 ATOM 1179 GLN 199 41.001 -4.419 CG 199 41.471 -3.266 6.742 1.00 0.00 3A4 MOTA 1180 CD GLN 6.348 1.00 0.00 3A4 GLN 199 42.353 -2.503 1181 OE1

ATOM

MOTA	1182	NE2	GLN	199	40.885	-3.125	7.963		0.00	3A4
MOTA	1183	C	GLN	199	40.319	-7.071	7.338	1.00	0.00	3A4
MOTA	1184	0	GLN	199	39.374	-6.533	7.889		0.00	3A4 3A4
ATOM	1185	N	ASP	200	40.193 38.939	-8.262 -8.983	6.717 6.597	1.00	0.00	3A4
ATOM	1186 1187	CA CB	ASP ASP	200 200	39.049 -		5.538	1.00	0.00	3A4
ATOM ATOM	1188	CG	ASP	200	37.683 -		5.079	1.00	0.00	3A4
ATOM	1189		ASP	200	37.459 -		5.238	1.00	0.00	3A4
ATOM	1190		ASP	200	36.855	-9.893	4.566	1.00	0.00	3A4
MOTA	1191	С	ASP	200	38.347	-9.432	7.927	1.00	0.00	3A4
MOTA	1192	0	ASP	200	37.137	-9.315	8.099	1.00	0.00	3A4
ATOM	1193	N	PRO	201	39.155	-9.847	8.917	1.00	0.00	3A4 3A4
MOTA	1194	CA	PRO	201	38.699 - 40.343 -		10.270 8.654	1.00	0.00	3A4
ATOM ATOM	1195 1196	CD CB	PRO PRO	201 201	39.936		11.012	1.00	0.00	3A4
ATOM	1197	CG	PRO	201	40.633		9.938	1.00	0.00	3A4
ATOM	1198	c	PRO	201	38.128	-8.916	10.997	1.00	0.00	3A4
ATOM	1199	0	PRO	201	37.076	-9.052	11.615	1.00	0.00	3A4
ATOM	1200	N	PHE	202	38.762	-7.733	10.872	1.00	0.00	3A4
MOTA	1201	CA	PHE	202	38.319	-6.521	11.530	1.00	0.00	3A4 3A4
ATOM	1202	СВ	PHE	202	39.462	-5.473 -5.259	11.494 12.888	1.00	0.00 0.00	3A4
ATOM	1203	CG	PHE PHE	202 202	40.009 40.365	-6.366	13.691	1.00	0.00	3A4
ATOM ATOM	1204 1205		PHE	202	40.293	-3.968	13.372	1.00	0.00	3A4
ATOM	1206		PHE	202	40.856	-6.184	14.987	1.00	0.00	3A4
ATOM	1207		PHE	202	40.855	-3.790	14.647	1.00	0.00	3A4
ATOM	1208	CZ	PHE	202	41.107	-4.894	15.465	1.00	0.00	3A4
ATOM	1209	C	PHE	202	37.080	-5.964	10.887	1.00	0.00	3A4 3A4
ATOM	1210	0	PHE	202	36.208	-5.444 -6.145	11.573 9.554	1.00	0.00	3A4
ATOM ATOM	1211	N CA	VAL VAL	203 203	36.928 35.752	-5.762	8.799	1.00	0.00	3A4
ATOM	1212 1213	CB	VAL	203	36.015	-5.808	7.287	1.00	0.00	3A4
ATOM	1214		VAL	203	34.738	-5.677	6.411	1.00	0.00	3A4
ATOM	1215		VAL	203	36.983	-4.648	6.954	1.00	0.00	3A4
ATOM	1216	С	VAL	203	34.545	-6.596	9.199	1.00	0.00	3A4
MOTA	1217	0	VAL	203	33.451	-6.068	9.364	1.00	0.00	3A4 3A4
ATOM	1218	N	GLU	204	34.736	-7.908 -8.782	9.475 9.967	1.00	0.00	3A4
ATOM ATOM	1219 1220	CA CB	GLU GLU	204 204	33.684 34.114	-10.262	9.912	1.00	0.00	3A4
ATOM	1221	CG	GLU	204		-10.797	8.472	1.00	0.00	3A4
ATOM	1222	CD	GLU	204		-12.210	8.489	1.00	0.00	3A4
ATOM	1223	OE1	GLU	204		-12.394	7.934	1.00	0.00	3A4
MOTA	1224		GLU	204		-13.123	9.059	1.00	0.00	3A4
MOTA	1225	C	GLU	204	33.230	-8.440 -8.449	11.373 11.666	1.00	0.00 0.00	3A4 3A4
ATOM	1226 1227	O N	GLU ASN	204 205	32.042 34.176	-8.057	12.259	1.00	0.00	3A4
ATOM ATOM	1228	CA	ASN	205	33.914	-7.660	13.628	1.00	0.00	3A4
ATOM	1229	СВ	ASN	205	35.248	-7.438	14.383	1.00	0.00	3A4
ATOM	1230	CG	ASN	205	36.015	-8.751	14.628	1.00	0.00	3A,4
MOTA	1231		LASN	205	37.233	-8.776	14.460	1.00	0.00	3A4
ATOM	1232		2 ASN	205	35.329	-9.842	15.069	1.00	0.00	3A4 3A4
MOTA MOTA	1233 1234	C O	ASN ASN	205 205	33.087 32.115	-6.395 -6.344	13.736 14.487	1.00	0.00	3A4
ATOM	1235	N	THR	206	33.414	-5.376	12.903		0.00	3A4
ATOM	1236	CA	THR	206	32.762	-4.077	12.899	1.00	0.00	3A4
ATOM	1237	СВ	THR	206	33.525	-3.007	12.102		0.00	3A4
MOTA	1238		1 THR	206	34.406	-3.549	11.139		0.00	3A4 3A4
ATOM	1239		2 THR	206	34.381	-2.246 -4.178	13.141			3A4
ATOM	1240	С 0	THR THR		31.364 30.435	-3.581	12.843			3A4
MOTA MOTA	1241 1242	N	LYS	200	31.178	-5.009	11.279			3A4
ATOM	1243	CA		207	29.905	-5.266	10.645			3A4
ATOM	1244	СВ	LYS		30.122	-6.061	9.349	1.00		3A4
MOTA	1245	CG	LYS	207	28.927	-6.211	8.393			3A4
ATOM	1246	CD			29.306	-6.802	7.027			3A4
MOTA	1247	CE			29.832	-8.246 -8.750	7.088 5.731			3A4 3A4
ATOM	1248	NZ	LYS		30.150 28.938	-8.750 -6.023	11.523			3A4
MOTA MOTA	1249 1250		LYS LYS		27.753	-5.736	11.533			3A4
ATOM	1251	N	LYS		29.441	-6.958	12.359			3A4
ATOM	1252			208	28.646	-7.727	13.293			3A4
ATOM	1253		LYS	208	29.443	-8.920	13.865	1.00	0.00	3A4

1.00 0.00 3A4 ATOM 1254 CG LYS 208 28.627 -9.993 14.610 1255 CD LYS 208 29.414 -11.248 15.031 1.00 0.00 3A4 MOTA 1.00 0.00 3A4 208 29.894 -12.177 13.900 1256 CE LYS ATOM 1.00 0.00 3A4 31.125 -11.677 13.236 NZ 208 ATOM 1257 LYS 0.00 14.430 1.00 3A4 MOTA 1258 С LYS 208 28.094 -6.905 0.00 208 26.931 -7.047 14.780 1.00 3A4 1259 0 LYS ATOM N LEU 209 28.886 -5.983 15.022 1.00 0.00 3A4 1260 ATOM 0.00 28.454 -5.149 16.133 1.00 3A4 209 ATOM 1261 CA LEU 29.656 -4.415 16.784 1.00 0.00 3A4 ATOM 1262 CB LEU 209 17.945 1.00 0.00 3A4 CG LEU 209 29.353 -3.397 **ATOM** 1263 28.592 -4.009 19.146 1.00 0.00 3A4 1264 CDI LEU 209 ATOM 30.596 1.00 0.00 3A4 209 -2.606 18.399 MOTA 1265 CD2 LEU -4.112 15.737 1.00 0.00 3A4 209 27,416 MOTA 1266 С LEU 26.515 1.00 0.00 3A4 MOTA 1267 0 LEU 209 -3.79316.507 3A4 210 27.527 -3.561 14.510 1.00 0.00 MOTA 1268 N LEU LEU 210 26.707 -2.449 14.080 1.00 0.00 3A4 MOTA 1269 CA 3A4 27.559 -1.343 13.418 1.00 0.00 CB LEU 210 MOTA 1270 -0.850 14.384 1.00 0.00 3A4 28.684 MOTA 1271 CG LEU 210 0.00 3A4 1272 CD1 LEU 210 29.655 0.113 13.699 1.00 ATOM 28.176 -0.257 15.717 1.00 0.00 3A4 ATOM 1273 CD2 LEU 210 25.611 -2.862 13.145 1.00 0.00 3A4 LEU 210 ATOM 1274 С 24.465 13.335 1.00 0.00 3A4 -2.454 ATOM 1275 O T.EU 210 3A4 0.00 25.948 -3.57112.035 1.00 ATOM 1276 N ARG 211 3A4 ATOM 1277 CA ARG 211 25.146 -3.650 10.816 1.00 0.00 26.033 -3.592 9.539 1.00 0.00 3A4 1278 CB ARG 211 ATOM 3A4 26.927 -2.337 9.503 1.00 0.00 1279 ARG 211 ATOM CG 27.841 0.00 3A4 -2.2208.274 1.00 ATOM 1280 CD ARG 211 3A4 1281 NE ARG 211 27.005 -2.107 7.024 1.00 0.00 ATOM 26.814 -0.939 6.329 1.00 0.00 3A4 1282 CZ ARG 211 ATOM 26.014 -0.951 5.223 1.00 0.00 3A4 ARG 211 1283 NH1 ATOM 27.397 0.236 6.711 1.00 0.00 3A4 ATOM 1284 NH2 ARG 211 0.00 3A4 24.236 -4.864 10.757 1.00 ATOM 1285 С ARG 211 0.00 3A4 1286 ARG 211 23.275 -4.868 9.989 1.00 ATOM 0 24.496 -5.910 11.589 1.00 0.00 3A4 1287 PHE 212 ATOM N 23.555 0.00 3A4 212 -6.992 11.826 1.00 ATOM 1288 CA PHE 3A4 23.730 -8.273 10.930 1.00 0.00 **ATOM** 1289 CB PHE 212 25.061 10.978 1.00 0.00 3A4 -8.998 MOTA 1290 CG PHE 212 25.170 -10.224 3A4 ATOM 1291 CD1 PHE 212 11.667 1.00 0.00 26.182 -8.527 10.268 1.00 0.00 3A4 ATOM 1292 CD2 PHE 212 1293 CE1 PHE 212 26.367 -10.954 11.660 1.00 0.00 3A4 ATOM 27.380 -9.259 10.254 1.00 0.00 3A4 PHE 212 ATOM 1294 CE2 0.00 3A4 27.474 -10.469 10.952 1.00 ATOM 1295 CZ PHE 212 3A4 0.00 ATOM 1296 С PHE 212 23.608 -7.246 13.314 1.00 1297 o PHE 212 24.292 -8.143 13.802 1.00 0.00 3A4 ATOM 0.00 3A4 ASP 213 22.863 -6.398 14.068 1.00 1298 N ATOM 22.843 -6.356 15.513 1.00 0.00 3A4 ASP ATOM 1299 CA 213 23.642 0.00 3A4 -5.131 1.00 ATOM 1300 CB ASP 213 16.046 3A4 ASP 213 23.916 -5.215 17.558 1.00 0.00 ATOM 1301 CG -6.179 3A4 24.608 17.982 1.00 0.00 ATOM 1302 OD1 ASP 213 3A4 OD2 ASP 23.444 -4.312 18.300 1.00 0.00 1303 213 ATOM 21.391 -6.281 15.902 1.00 0.00 3A4 ATOM 1304 С ASP 213 3A4 -5.286 15.648 1.00 0.00 ATOM 1305 0 ASP 213 20.714 3A4 PHE 214 20.894 -7.371 16.533 1.00 0.00 ATOM 1306 N 19.516 -7.516 16.941 1.00 0.00 3A4 1307 CA PHE 214 ATOM PHE 18.526 -7.900 15.776 1.00 0.00 3A4 ATOM 1308 CB 214 19.127 -8.826 14.734 1.00 0.00 3A4 PHE ATOM 1309 CG 214 0.00 3A4 -8.306 13.515 1.00 MOTA 1310 CD1 PHE 214 19.610 3A4 CD2 PHE 214 19.216 -10.215 14.950 1.00 0.00 **ATOM** 1311 -9.143 12.550 1.00 0.00 3A4 ATOM 1312 CE1 PHE 214 20.186 19.793 -11.058 13.987 1.00 0.00 3A4 CE2 PHE 214 ATOM 1313 20.280 -10.520 12.788 1.00 0.00 3A4 MOTA 1314 CZ PHE 214 3A4 18.034 1,00 0.00 ATOM 1315 С PHE 214 19.513 -8.554 3A4 ATOM 1316 0 PHE 214 20.344 -9.460 18.058 1.00 0.00 18.527 18.956 1.00 0.00 3A4 ATOM 1317 N LEU 215 -8.428 0.00 3A4 18.216 -9.384 19.995 1.00 CA LEU 215 ATOM 1318 3A4 -9.072 21.353 1.00 0.00 LEU 18.914 ATOM 1319 CB 215 3A4 18.685 -10.089 1.00 0.00 ATOM 1320 CG LEU 215 22.505 1321 CD1 LEU 215 19.075 -11.533 22,128 1.00 0.00 3A4 MOTA 19.419 23.783 1.00 0.00 3A4 CD2 LEU 215 -9.639 ATOM 1322 16.716 -9.298 20.078 1.00 0.00 3A4 LEU 215 MOTA 1323 C 20.970 1.00 0.00 3A4 16.151 -8.667 MOTA 1324 0 LEU 215 19.073 1.00 0.00 3A4 1325 N ASP 216 16.046 -9.926 ATOM

ATOM	1326	CA	ASP	216	14.627	-9.830	18.781	1.00	0.00	3A4
MOTA	1327	СВ	ASP	216		-9.623	17.242	1.00	0.00	3A4
MOTA	1328	CG	ASP	216	14.915 -		16.328	1.00	0.00	3A4 3A4
ATOM	1329	OD1 OD2		216 216	16.161 - 14.075 -		16.241 15.700	1.00	0.00	3A4
ATOM ATOM	1330 1331	C	ASP	216	13.914 -		19.316	1.00	0.00	3A4
ATOM	1332	ŏ	ASP	216	14.578 -		19.506	1.00	0.00	3A4
ATOM	1333	N	PRO	217	12.576 -		19.553	1.00	0.00	3A4
MOTA	1334	CA	PRO	217	11.794 -		19.974	1.00	0.00	3A4
ATOM	1335	CD	PRO	217	11.814	-9.819	19.695	1.00	0.00	3A4
MOTA	1336	CB	PRO	217	10.525 - 10.367 -		20.611	1.00 1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1337 1338	CG CG	PRO PRO	217 217	11.504 -		18.786	1.00	0.00	3A4
ATOM	1339	ŏ	PRO	217	12.309 -		18.527	1.00	0.00	3A4
ATOM	1340	N	PHE	218	10.374 -		18.064	1.00	0.00	3A4
ATOM	1341	CA	PHE	218	10.004 -		16.839	1.00	0.00	3A4
ATOM	1342	СВ	PHE	218	8.877 -		17.032	1.00	0.00	3A4
ATOM	1343	CG	PHE	218	9.294 - 8.630 -		18.036 19.273	1.00 1.00	0.00	3A4 3A4
MOTA MOTA	1344 1345		PHE PHE	218 218	10.354		17.766	1.00	0.00	3A4
ATOM	1346		PHE	218	9.018		20.225	1.00	0.00	3A4
ATOM	1347		PHE	218	10.751 -		18.720	1.00	0.00	3A4
MOTA	1348	CZ	PHE	218	10.083		19.950	1.00	0.00	3A4
MOTA	1349	С	PHE	218		-12.564	15.883	1.00	0.00	3A4
ATOM	1350	0	PHE	218		-12.860	14.737	1.00	0.00	3A4 3A4
ATOM	1351	N	PHE	219 219		-11.297 -10.165	16.374 15.736	1.00 1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1352 1353	CA CB	PHE	219		-9.630	16.572	1.00	0.00	3A4
ATOM	1354	CG	PHE	219		-10.646	16.570	1.00	0.00	3A4
ATOM	1355		PHE	219		-10.600	15.587	1.00	0.00	3A4
ATOM	1356		PHE	219		-11.664	17.542	1.00	0.00	3A4
ATOM	1357		PHE	219		-11.546	15.576	1.00	0.00	3A4
ATOM	1358		PHE	219		-12.611 -12.551	17.536 16.553	1.00	0.00	3A4 3A4
ATOM ATOM	1359 1360	CZ C	PHE	219 219	9.798	-9.078	15.602	1.00	0.00	3A4
ATOM	1361	Ö	PHE	219	10.805	-9.068	16.307	1.00	0.00	3A4
ATOM	1362	N	LEU	220	9.547	-8.131	14.664	1.00	0.00	3A4
MOTA	1363	CA	LEU	220	10.447	-7.050	14.321	1.00	0.00	3A4
ATOM	1364	CB	LEU	220	11.550	-7.452	13.279	1.00	0.00	3A4
MOTA	1365	CG	LEU	220	11.130 12.368	-7.889 -7.938	11.840 10.924	1.00 1.00	0.00	3A4 3A4
MOTA MOTA	1366 1367		LEU	220 220	10.365	-9.229	11.764	1.00	0.00	3A4
ATOM	1368	c	LEU	220	9.590	-5.908	13.825	1.00	0.00	3A4
ATOM	1369	O	LEU	220	8.366	-5.964	13.937	1.00	0.00	3A4
MOTA	1370	N	SER	221	10.268	-4.849	13.284	1.00	0.00	3A4
MOTA	1371	CA	SER	221	9.781	-3.584	12.735	1.00	0.00	3A4 3A4
MOTA	1372	CB	SER	221 221	8.270 7.980	-3.542 -2.485	12.288 11.376	1.00	0.00	3A4
ATOM ATOM	1373 1374	OG C	SER SER	221	10.129	-2.514	13.764	1.00	0.00	3A4
ATOM	1375	ŏ	SER	221	10.958	-2.740	14.646	1.00	0.00	3A4
MOTA	1376	N	ILE	222	9.495	-1.312	13.661	1.00	0.00	3A4
MOTA	1377	CA	ILE	222	9.692	-0.155	14.524	1.00	0.00	3A4 3A4
ATOM	1378	CB	ILE	222	9.886	1.145	13.735 13.025	1.00	0.00	3A4 3A4
ATOM ATOM	1379 1380		ILE ILE	222 222	11.258 8.727	1.449	12.741	1.00	0.00	3A4
MOTA	1381	CD	ILE	222	8.868	2.791	12.016	1.00	0.00	3A4
ATOM	1382	c	ILE	222	8.533	-0.038	15.500	1.00	0.00	3A4
MOTA	1383	0	ILE	222	8.631	0.670	16.501	1.00	0.00	3A4
MOTA	1384	N	THR	223	7.406	-0.746	15.215		0.00	3A4
MOTA	1385	CA	THR	223	6.225	-0.787	16.050		0.00	3A4 3A4
ATOM	1386	CB	THR	223 223	5.259 4.159	0.384 0.414	15.782 16.691		0.00	3A4
ATOM ATOM	1387 1388		THR	223	4.751	0.419	14.318		0.00	3A4
ATOM	1389	c c	THR	223	5.633	-2.165	15.811		0.00	3A4
MOTA	1390		THR	223	5.360	-2.558	14.678		0.00	3A4
MOTA	1391	N	VAL	224	5.435	-2.927	16.918		0.00	3A4
ATOM	1392	CA	VAL	224	4.832	-4.244	16.917		0.00	3A4 3A4
ATOM	1393		VAL	224 224	5.751 7.065	-5.354 -5.517	16.379 17.186		0.00	3A4
MOTA MOTA	1394 1395		L VAL	224	4.973	-6.679	16.198			3A4
ATOM	1396		VAL	224	4.397	-4.468	18.349			3A4
ATOM	1397		VAL	224	5.085	-4.071	19.290	1.00	0.00	3A4

ATOM	1398	N	PHE	225	3.212	-5.114	18.534	1.00	0.00	3A4
MOTA	1399	CA	PHE	225	2.568	-5.398	19.809	1.00	0.00	3A4
ATOM	1400	СВ	PHE	225	1.025	-5.112	19.736	1.00	0.00	3A4 3A4
MOTA MOTA	1401 1402	CG CD1	PHE	225 225	0.345 0.584	-5.089 -4.036	21.089 21.993	1.00	0.00	3A4
ATOM	1402	CD2		225	-0.533	-6.123	21.470	1.00	0.00	3A4
ATOM	1404	CE1		225	-0.038	-4.017	23.251	1.00	0.00	3A4
MOTA	1405	CE2	PHE	225	-1.156	-6.107	22.726	1.00	0.00	3A4
MOTA	1406	CZ	PHE	225	-0.908	-5.053	23.617	1.00	0.00	3A4
ATOM	1407	C	PHE	225	2.898	-6.812	20.313	1.00	0.00	3A4 3A4
ATOM ATOM	1408 1409	O N	PHE PRO	225 226	3.306 2.776	-6.885 -7.964	21.472 19.590	1.00	0.00	3A4 3A4
ATOM	1410	CA	PRO	226	3.087	-9.298	20.117	1.00	0.00	3A4
ATOM	1411	CD	PRO	226	2.027	-8.062	18.335	1.00	0.00	3A4
MOTA	1412	СВ	PRO	226		-10.268	19.186	1.00	0.00	3A4
MOTA	1413	CG	PRO	226	2.191	-9.507	17.865	1.00	0.00	3A4
ATOM	1414	C	PRO	226	4.587	-9.598	20.127	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	1415 1416	O N	PRO PHE	226 227	5.346 4.993	-9.003 -10.544	19.361 21.009	1.00	0.00	3A4
ATOM	1417	CA	PHE	227		-10.995	21.212	1.00	0.00	3A4
MOTA	1418	СВ	PHE	227		-10.254	22.376	1.00	0.00	3A4
MOTA	1419	CG	PHE	227	6.298	-10.129	23.651	1.00	0.00	3A4
MOTA	1420		PHE	227	5.437	-9.031	23.855	1.00	0.00	3A4
ATOM	1421		PHE	227		-11.105	24.663	1.00	0.00	3A4
MOTA	1422		PHE	227 227	4.677	-8.920 -10.999	25.028 25.838	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1423 1424	CZ	PHE	227	4.775	-9.907	26.019	1.00	0.00	3A4
ATOM	1425	c	PHE	227		-12.495	21.429	1.00	0.00	3A4
ATOM	1426	0	PHE	227	7.291	-13.188	21.177	1.00	0.00	3A4
MOTA	1427	N	LEU	228		-13.001	21.925	1.00	0.00	3A4
MOTA	1428	CA	LEU	228		-14.389	22.186	1.00	0.00	3A4
ATOM ATOM	1429 1430	CB CG	LEU	228 228		-15.381 -16.607	21.024 20.757	1.00	0.00	3A4 3A4
ATOM	1431		LEU	228		-17.707	21.832	1.00	0.00	3A4
ATOM	1432		LEU	228		-16.215	20.406	1.00	0.00	3A4
ATOM	1433	С	LEU	228	5.274	-14.788	23.565	1.00	0.00	3A4
ATOM	1434	0	LEU	228		-14.291	24.575	1.00	0.00	3A4
MOTA	1435	N	ILE	229		-15.659	23.623	1.00	0.00	3A4 3A4
MOTA MOTA	1436 1437	CA CB	ILE	229 229		-15.948 -16.944	24.811 25.799	1.00	0.00	3A4
ATOM	1438		ILE	229		-18.311	25.188	1.00	0.00	3A4
ATOM	1439		ILE	229	7.185	-17.043	27.173	1.00	0.00	3A4
MOTA	1440	CD	ILE	229		-18.014	27.278	1.00	0.00	3A4
MOTA	1441	С	ILE	229		-16.351	24.252	1.00	0.00	3A4 3A4
ATOM ATOM	1442 1443	О И	ILE PRO	229 230		-17.503 -15.455	23.857 24.157	1.00	0.00	3A4
ATOM	1444	CA	PRO	230		-15.735	23.519	1.00	0.00	3A4
ATOM	1445	CD	PRO	230		-14.022	24.410	1.00	0.00	3A4
ATOM	1446	CB	PRO	230		-14.349	23.055	1.00	0.00	3A4
MOTA	1447	CG	PRO	230		-13.376	24.082	1.00	0.00	3A4
ATOM	1448 1449	C O	PRO	230 230		-16.380 -16.422	24.483 25.691	1.00	0.00	3A4 3A4
ATOM ATOM	1450	N	PRO ILE	231		-16.870	23.931	1.00	0.00	3A4
ATOM	1451	CA	ILE	231		-17.495	24.644	1.00	0.00	3A4
ATOM	1452	СВ	ILE	231		-18.802	23.988	1.00	0.00	3A4
MOTA	1453		ILE	231		-19.489	24.852	1.00	0.00	3A4
ATOM	1454		ILE	231		-19.767	23.714	1.00	0.00	3A4
ATOM ATOM	1455 1456	CD C	ILE	231 231		-20.240 -16.473	24.953 24.709	1.00	0.00	3A4 3A4
ATOM	1457	o	ILE	231		-16.247	25.773	1.00	0.00	3A4
ATOM	1458	N	LEU	232		-15.844	23.533	1.00	0.00	3A4
ATOM	1459	CA	LEU	232	16.397	-14.778	23.277	1.00	0.00	3A4
MOTA	1460	СВ	LEU	232		-13.552	24.250	1.00	0.00	3A4
ATOM	1461	CG	LEU	232		-12.824	24.269	1.00	0.00	3A4 3A4
MOTA MOTA	1462 1463		LEU LEU	232 232		-11.763 -12.203	25.383 22.908	1.00	0.00	3A4 3A4
ATOM	1464	CDZ	LEU			-15.328	23.232	1.00	0.00	3A4
ATOM	1465	ŏ	LEU			-15.133	24.154	1.00	0.00	3A4
ATOM	1466	N	GLU	233	18.131	-16.047	22.125	1.00	0.00	3A4
ATOM	1467	CA	GLU			-16.728	21.896		0.00	3A4
ATOM	1468	CB	GLU			-18.268	22.115	1.00	0.00	3A4
MOTA	1469	CG	GLU	233	18.095	-18.955	21.373	1.00	0.00	3A4

ATOM	1470	CD	GLU	233	18.120 -2	20.462	21.648	1.00	0.00	3A4
ATOM	1471	OE1		233	19.140 -2	21.114	21.295	1.00	0.00	3A4
ATOM	1472		GLU	233	17.118 -2		22.205	1.00	0.00	3A4
ATOM	1473		GLU	233	19.828 -		20.489	1.00	0.00	3A4
ATOM	1474		GLU	233	20.256 -		19.726	1.00	0.00	3A4
				234	19.734 -		20.125	1.00	0.00	3A4
ATOM	1475	N	VAL				18.815	1.00	0.00	3A4
ATOM	1476	CA	VAL	234	20.053 -			1.00	0.00	3A4
MOTA	1477	СВ	VAL	234	18.792 -		17.987			3A4
ATOM	1478	CG1		234	17.739 -		18.723	1.00	0.00	
ATOM	1479	CG2	VAL	234	19.142 -		16.568	1.00	0.00	3A4
MOTA	1480	C	VAL	234	20.960 -	13.370	19.064	1.00	0.00	3A4
MOTA	1481	0	VAL	234	20.563 -	12.209	18.984	1.00	0.00	3A4
ATOM	1482	N	LEU	235	22.242 -	13.673	19.393	1.00	0.00	3A4
MOTA	1483	CA	LEU	235	23.270 -	12.694	19.675	1.00	0.00	3A4
ATOM	1484	СВ	LEU	235	23.137 -	11.954	21.056	1.00	0.00	3A4
ATOM	1485	CG	LEU	235	23.294 -	12.749	22.393	1.00	0.00	3A4
ATOM	1486	CD1		235	23.236 -		23.594	1.00	0.00	3A4
ATOM	1487		LEU	235	22.289 -		22.600	1.00	0.00	3A4
			LEU	235	24.592 ~		19.593	1.00	0.00	3A4
ATOM	1488	C			24.703 -		19.948	1.00	0.00	3A4
ATOM	1489	0	LEU	235				1.00	0.00	3A4
ATOM	1490	N	ASN	236	25.638 -		19.128			3A4
MOTA	1491	CA	ASN	236	27.013 -		19.089	1.00	0.00	
MOTA	1492	CB	ASN	236	27.351 -		17.803	1.00	0.00	3A4
ATOM	1493	CG	ASN	236	28.697 -		17.931	1.00	0.00	3A4
MOTA	1494	OD1	ASN	236	28.818 -	15.613	18.753	1.00	0.00	3A4
MOTA	1495	ND2	ASN	236	29.719 -	14.326	17.115	1.00	0.00	3A4
ATOM	1496	С	ASN	236	27.795 -	11.845	19.165	1.00	0.00	3A4
MOTA	1497	0	ASN	236	28.546 -	11.489	18.259	1.00	0.00	3A4
ATOM	1498	N	ILE	237	27.590 -	11.096	20.283	1.00	0.00	3A4
ATOM	1499	CA	ILE	237	28.074	-9.747	20.504	1.00	0.00	3A4
ATOM	1500	СВ	ILE	237	26.980	-8.800	20.998	1.00	0.00	3A4
ATOM	1501		ILE	237	26.039	-8.584	19.789	1.00	0.00	3A4
	1502		ILE	237	26.203	-9.271	22.262	1.00	0.00	3A4
ATOM				237	25.059	-8.341	22.671	1.00	0.00	3A4
ATOM	1503	CD	ILE			-9.798		1.00	0.00	3A4
ATOM	1504	Ç	ILE	237	29.228		21.461			3A4
ATOM	1505	0	ILE	237	30.202	-9.126	21.226	1.00	0.00	
ATOM	1506	N	CYS	238	29.124 -		22.532	1.00	0.00	3A4
MOTA	1507	CA	CYS	238	30.099 -		23.576	1.00	0.00	3A4
ATOM	1508	CB	CYS	238	29.513 -		24.739	1.00	0.00	3A4
MOTA	1509	SG	CYS	238	28.106 -		25.526	1.00	0.00	3A4
ATOM	1510	С	CYS	238	31.307 -	-11.563	23.083	1.00	0.00	3A4
ATOM	1511	0	CYS	238	32.424 -	-11.278	23.493	1.00	0.00	3A4
ATOM	1512	N	VAL	239	31.138 -	-12.446	22.082	1.00	0.00	3A4
ATOM	1513	CA	VAL	239	32.219 -	-13.161	21.438	1.00	0.00	3A4
ATOM	1514	CB.	VAL	239	31.700 -		20.675	1.00	0.00	3A4
ATOM	1515		VAL	239	32.858		20.247	1.00	0.00	3A4
ATOM	1516		VAL	239	30.715		21.586	1.00	0.00	3A4
ATOM	1517	c	VAL	239	33.006		20.505	1.00	0.00	3A4
	1518	ŏ	VAL	239	34.228		20.485	1.00	0.00	3A4
ATOM	1519			240	32.315		19.731	1.00	0.00	3A4
ATOM		И	PHE	240	32.913		18.870	1.00	0.00	3A4
ATOM	1520	CA	PHE		31.825			1.00	0.00	3A4
ATOM	1521	CB	PHE	240		-9.669	18.040			3A4
ATOM	1522	CG	PHE	240	31.881	-8.134	17.899	1.00	0.00	3A4
ATOM	1523		PHE	240	32.913	-7.550	17.149	1.00	0.00	
ATOM	1524		PHE	240	31.185	-7.320	18.812	1.00	0.00	3A4
MOTA	1525	CE1	PHE	240	33.312	-6.223	17.382	1.00	0.00	3A4
ATOM	1526	CE2	PHE	240	31.646	-6.034	19.117	1.00	0.00	3A4
ATOM	1527	CZ	PHE	240	32.709	-5.481	18.396	1.00	0.00	3A4
MOTA	1528	С	PHE	240	33.789	-9.440	19.608	1.00	0.00	3A4
ATOM	1529	0	PHE	240	34.906	-9.202	19.168	1.00	0.00	3A4
ATOM	1530	N	PRO	241	33.347	-8.835	20.727	1.00	0.00	3A4
ATOM	1531	CA	PRO	241	34.111	-7.940	21.493	1.00	0.00	3A4
ATOM	1532	CD	PRO	241	32.648	-9.345	21.724	1.00	0.00	3A4
ATOM			PRO		33.196	-7.358	22.578	1.00	0.00	3A4
	1533	CB			32.348	-8.435	22.936		0.00	3A4
ATOM	1534	CG	PRO				22.936			3A4
ATOM	1535	C	PRO		35.347	-8.605				3A4
ATOM	1536	0	PRO		36.396	-7.992	22.029			3A4
MOTA	1537	N	ARG		35.316	-9.867	22.592			
MOTA	1538	CA	ARG			-10.583				3A4
MOTA	1539	СВ	ARG			-11.889				3A4
MOTA	1540	CG	ARG			-11.657				3A4
ATOM	1541	CD	ARG	242	34.515	-12.928	25.556	1.00	0.00	3A4

ATOM	1542	NE	ARG	242	33.717 -	-12.581	26.784		0.00	3A4
MOTA	1543	CZ	ARG	242	32.762 -		27.314		0.00	3A4
ATOM	1544	NH1		242	32.114 -		28.455		0.00	3A4 3A4
ATOM	1545	NH2		242	32.444 - 37.483 -		26.725 22.037	1.00	0.00	3A4
ATOM	1546 1547	С 0	ARG ARG	242 242	38.677 -		22.298	1.00	0.00	3A4
MOTA MOTA	1548	N	GLU	243	37.044		20.784	1.00	0.00	3A4
ATOM	1549	CA	GLU	243	37.911 -		19.638	1.00	0.00	3A4
ATOM	1550	СВ	GLU	243	37.126		18.383	1.00	0.00	3A4
ATOM	1551	CG	GLU	243	36.626		18.452	1.00	0.00	3A4
MOTA	1552	CD	GLU	243	35.759	-13.581	17.219	1.00	0.00	3A4
ATOM	1553		GLU	243	34.528		17.385	1.00	0.00	3A4
MOTA	1554		GLU	243	36.319		16.089	1.00	0.00	3A4 3A4
ATOM	1555	C	GLU	243	38.703		19.275 19.057	1.00	0.00	3A4
ATOM	1556	0	GLU	243 244	39.908 38.043	-8.981	19.037	1.00	0.00	3A4
ATOM ATOM	1557 1558	N CA	VAL VAL	244	38.684	-7.714	18.990	1.00	0.00	3A4
ATOM	1559	СВ	VAL	244	37.676	-6.607	18.731	1.00	0.00	3A4
ATOM	1560		VAL	244	38.391	-5.314	18.259	1.00	0.00	3A4
ATOM	1561		VAL	244	36.813	-7.052	17.545	1.00	0.00	3A4
ATOM	1562	С	VAL	244	39.649	-7.327	20.084	1.00	0.00	3A4
MOTA	1563	0	VAL	244	40.771	-6.912	19.811	1.00	0.00	3A4
MOTA	1564	N	THR	245	39.257	-7.535	21.357	1.00	0.00	3A4
ATOM	1565	CA	THR	245	40.070	-7.264	22.527	1.00	0.00	3A4
ATOM	1566	СВ	THR	245	39.245	-7.434	23.795	1.00	0.00	3A4 3A4
ATOM	1567		THR	245	38.211	-6.455	23.817 25.127	1.00	0.00 0.00	3A4 3A4
ATOM	1568	CG2	THR THR	245 245	40.041 41.317	-7.330 -8.113	22.572	1.00	0.00	3A4
MOTA MOTA	1569 1570	ŏ	THR	245	42.397	-7.605	22.842	1.00	0.00	3A4
ATOM	1571	N	ASN	246	41.225	-9.408	22.207	1.00	0.00	3A4
ATOM	1572	CA	ASN	246		-10.327	22.152	1.00	0.00	3A4
ATOM	1573	СВ	ASN	246	41.877	-11.774	21.874	1.00	0.00	3A4
ATOM	1574	CG	ASN	246		-12.349	23.082	1.00	0.00	3A4
MOTA	1575		ASN	246		-11.808	24.187	1.00	0.00	3A4
MOTA	1576		ASN	246		-13.502	22.862	1.00	0.00	3A4 3A4
ATOM	1577	C	ASN	246		-9.950 -10.003	21.088 21.305	1.00	0.00	3A4
MOTA	1578	O N	ASN PHE	246 247	42.846	-9.491	19.921	1.00	0.00	3A4
ATOM ATOM	1579 1580	CA	PHE	247	43.640	-9.006	18.820	1.00	0.00	3A4
ATOM	1581	СВ	PHE	247	42.712	-8.691	17.625	1.00	0.00	3A4
ATOM	1582	CG	PHE	247	43.520	-8.335	16.378	1.00	0.00	3A4
ATOM	1583	CD1	PHE	247	44.084	-9.348	15.580	1.00	0.00	3A4
MOTA	1584		PHE	247	43.817	-6.990	16.065	1.00	0.00	3A4
MOTA	1585		PHE	247	44.943	-9.028	14.517	1.00	0.00	3A4 3A4
MOTA	1586		PHE	247	44.673	-6.665	15.008 14.243	1.00	0.00	3A4
ATOM	1587	CZ C	PHE	247 247	45.245 44.438	-7.686 -7.768	19.171	1.00	0.00	3A4
MOTA MOTA	1588 1589	Ö	PHE	247	45.631	-7.693	18.897	1.00	0.00	3A4
ATOM	1590	N	LEU	248	43.781	-6.766	19.795	1.00	0.00	. 3A4
ATOM	1591	CA	LEU	248	44.374	-5.480	20.131	1.00	0.00	3A4
ATOM	1592	CB	LEU	248	43.291	-4.473	20.599	1.00	0.00	3A4
MOTA	1593	CG	LEU	248	42.423	-3.985	19.422	1.00	0.00	3A4
MOTA	1594		LEU	248	41.143	-3.318	19.920	1.00	0.00	3A4
ATOM	1595		LEU		43.179		18.448	1.00	0.00	3A4 3A4
ATOM	1596	C	LEU	248	45.407 46.458		21.219 21.175	1.00	0.00	3A4
ATOM ATOM	1597 1598	N N	LEU ARG		45.152					3A4
ATOM	1599	CA	ARG		46.055		23.263	1.00		3A4
ATOM	1600	СВ	ARG		45.402					3A4
MOTA	1601	CG	ARG		44.526			1.00	0.00	3A4
ATOM	1602	CD	ARG		45.372	-6.731	26.426	1.00		3A4
MOTA	1603	NE	ARG	249	44.462					3A4
MOTA	1604	ÇZ	ARG		44.932					3A4
ATOM	1605		1 ARG		44.068					3A4
ATOM	1606		2 ARG		46.251					3A4 3A4
ATOM	1607		ARG		47.418					3A4
MOTA MOTA	1608 1609		ARG LYS		48.444 47.456					3A4
MOTA	1610				48.664					3A4
ATOM	1611				48.353					3A4
ATOM	1612					-11.007		1.00		3A4
ATOM	1613				47.184	-11.995	19.759	1.00	0.00	3A4

MOTA	1614	CE	LYS	250	46.472	-13.190	20.404	1.00	0.00	3A4
ATOM	1615	NZ	LYS	250		-14.102	19.372	1.00	0.00	3A4
ATOM	1616	C	LYS	250	49.481	-7.572	20.506	1.00	0.00	3A4
ATOM	1617	0	LYS	250	50.699	-7.572	20.583	1.00	0.00	3A4
ATOM	1618	N	SER	251	48.809	-6.584	19.881	1.00	0.00	3A4
ATOM	1619	CA	SER	251	49.413	-5.423	19.268	1.00	0.00	3A4
ATOM	1620	СВ	SER	251	48.350	-4.598	18.498	1.00	0.00	3A4
ATOM	1621	OG	SER	251	47.705	-5.410	17.524	1.00	0.00	3A4
ATOM	1622	С	SER	251	50.056	-4.492	20.271	1.00	0.00	3A4
MOTA	1623	0	SER	251	51.163	-4.000	20.091	1.00	0.00	3A4
ATOM	1624	N	VAL	252	49.376		21.416	1.00	0.00	3A4
ATOM	1625	CA	VAL	252	49.809		22.495	1.00	0.00	3A4
MOTA	1626	СВ	VAL	252	48.673		23.486	1.00	0.00	3A4
ATOM	1627		VAL	252	49.132		24.775	1.00	0.00	3A4
ATOM	1628		VAL	252	47.610		22.625	1.00	0.00	3A4 3A4
ATOM	1629	C	VAL	252	51.052		23.163	1.00	0.00	3A4
ATOM	1630	0	VAL	252	51.998		23.419	1.00	0.00	3A4
ATOM	1631	N	LYS	253	51.108		23.380 23.944	1.00	0.00	3A4
ATOM	1632	CA	LYS	253	52.243 51.887		24.155	1.00	0.00	3A4
MOTA	1633	CB	LYS	253	52.903		24.153	1.00	0.00	3A4
ATOM	1634	CG	LYS	253 253	52.410		25.224	1.00	0.00	3A4
MOTA MOTA	1635 1636	CD CE	LYS LYS	253		-10.563	26.018	1.00	0.00	3A4
ATOM	1637	NZ	LYS	253		-11.929	26.256	1.00	0.00	3A4
ATOM	1638	C	LYS	253	53.481		23.082	1.00	0.00	3A4
ATOM	1639	ō	LYS	253	54.570		23.557	1.00	0.00	3A4
ATOM	1640	N	ARG	254	53.316		21.752	1.00	0.00	3A4
ATOM	1641	CA	ARG	254	54.372		20.768	1.00	0.00	3A4
ATOM	1642	СВ	ARG	254	53.887		19.369	1.00	0.00	3A4
ATOM	1643	CG	ARG	254	53.631	-7.877	19.278	1.00	0.00	3A4
ATOM	1644	CD	ARG	254	52.822	-8.252	18.031	1.00	0.00	3A4
MOTA	1645	NE	ARG	254	52.473	-9.714	18.098	1.00	0.00	3A4
MOTA	1646	CZ	ARG	254	51.381	-10.256	17.466	1.00	0.00	3A4
MOTA	1647	NHl	ARG	254		-11.591	17.596	1.00	0.00	3A4
ATOM	1648	NH2	ARG	254	50.529		16.721	1.00	0.00	3A4
ATOM	1649	С	ARG	254	54.899		20.676	1,.00	0.00	3A4
ATOM	1650	0	ARG	254	56.093		20.498	1.00	0.00	3A4
ATOM	1651	N	MET	255	54.021		20.844	1.00	0.00	3A4
ATOM	1652	CA	MET	255	54.372		20.777	1.00	0.00	3A4
ATOM	1653	CB	MET	255	53.141		20.406	1.00	0.00	3A4 3A4
ATOM	1654	CG	MET	255	52.816		18.917 18.447	1.00	0.00	3A4
ATOM	1655 1656	SD CE	MET	255 255	51.250 51.470		16.649	1.00	0.00	3A4
ATOM ATOM	1657	CE	MET MET	255	55.008		22.041	1.00	0.00	3A4
ATOM	1658	ò	MET	255	55.687		22.027	1.00	0.00	3A4
ATOM	1659	N	LYS	256	54.853		23.174	1.00	0.00	3A4
ATOM	1660	CA	LYS	256	55.524		24.424	1.00	0.00	3A4
ATOM	1661	СВ	LYS	256	54.809		25.623	1.00	0.00	3A4
ATOM	1662	CG	LYS	256	53.53		26.076	1.00	Q.00	3A4
ATOM	1663	CD	LYS	256	52.72	6 -2.649	27.168	1.00	0.00	3A4
ATOM	1664	CE	LYS	256	53.383	3 -2.616	28.556	1.00	0.00	3A4
ATOM	1665	NZ	LYS	256	52.48	7 -3.206		1.00	0.00	3A4
MOTA	1666	С	LYS	256	56.96		24.397	1.00	0.00	3A4
ATOM	1667	0	LYS	256	57.83		25.029	1.00	0.00	3A4
ATOM	1668	N	GLU	257	57.22		23.619	1.00	0.00	3A4
MOTA	1669	CA	GLU	257	58.52		23.444	1.00	0.00	3A4
MOTA	1670	CB	GLU	257	58.42		23.058		0.00	3A4
ATOM	1671	CG	GLU	257	57.81				0.00	3A4 3A4
ATOM	1672	CD	GLU	257	57.60				0.00	3A4
ATOM	1673		GLU	257	56.42 58.62				0.00	3A4
ATOM	1674		GLU	257 257	59.38				0.00	3A4
MOTA MOTA	1675 1676	c o	GTN GTN	257	60.40				0.00	3A4
ATOM	1677	N	SER		59.00				0.00	3A4
ATOM	1678	CA	SER		59.76					3A4
MOTA	1679	CB	SER		61.18					3A4
ATOM	1680	OG	SER		62.00					3A4
ATOM	1681	c	SER		58.93					3A4
ATOM	1682	Ō	SER		58.50			1.00		3A4
ATOM	1683	N	ARG		58.77	9 -2.011				3A4
ATOM	1684	CA	ARG		58.39					3A4
ATOM	1685	CB	ARG	259	56.88	0 -1.758	16.329	1.00	0.00	3A4

MOTA	1686	CG	ARG	259	55.968	-2.939	16.688	1.00	0.00	3A4
ATOM	1687		ARG	259		-2.858	15.987	1.00	0.00	3A4
ATOM	1688		ARG	259		-4.000	16.458	1.00	0.00 0.00	3A4 3A4
ATOM	1689		ARG	259 259		-4.411 -5.390	15.791 16.332	1.00	0.00	3A4
MOTA MOTA	1690 1691	NH1 NH2		259	52.247	-3.859	14.598	1.00	0.00	3A4
ATOM	1692	C	ARG	259	59.262	-0.943	16.000	1.00	0.00	3A4
ATOM	1693	0	ARG	259	60.401	-1.220	15.626	1.00	0.00	3A4
MOTA	1694	N	LEU	260	58.752	0.314	15.898	1.00	0.00	3A4
ATOM	1695	CA	LEU	260	59.502	1.436	15.373	1.00	0.00 0.00	3A4 3A4
MOTA	1696	CB	LEU	260 260	59.602 60.595	1.425 2.428	13.811 13.175	1.00	0.00	3A4
ATOM ATOM	1697 1698	CG CD1	LEU	260	62.054	2.163	13.599	1.00	0.00	3A4
ATOM	1699	CD2		260	60.467	2.427	11.640	1.00	0.00	3A4
ATOM	1700	С	LEU	260	58.790	2.670	15.874	1.00	0.00	3A4
MOTA	1701	0	LEU	260	58.005	3.291	15.159	1.00	0.00	3A4
ATOM	1702	N	GLU	261	59.062	3.038	17.155	1.00	0.00	3A4 3A4
ATOM	1703	CA	GLU	261 261	58.441 57.742	4.130 3.683	17.884 19.213	1.00	0.00	3A4
MOTA MOTA	1704 1705	CB CG	GLU	261	58.554	2.841	20.229	1.00	0.00	3A4
ATOM	1706	ÇD	GLU	261	58.717	1.386	19.761	1.00	0.00	3A4
ATOM	1707	OE1	GLU	261	59.884	0.942	19.589	1.00	0.00	. 3A4
MOTA	1708		GLU	261	57.675	0.701	19.572	1.00	0.00	3A4
ATOM	1709	С	GLU	261	59.482	5.186	18.166	1.00	0.00 0.00	3A4 3A4
ATOM	1710	O N	GLU ASP	261 262	60.619 59.067	4.877 6.478	18.523 17.991	1.00	0.00	3A4
ATOM ATOM	1711 1712	N CA	ASP	262	59.771	7.738	18.239	1.00	0.00	3A4
ATOM	1713	СВ	ASP	262	60.392	7.859	19.674	1.00	0.00	3A4
ATOM	1714	CG	ASP	262	59.293	7.671	20.735	1.00	0.00	3A4
MOTA	1715		ASP	262	59.392	6.700	21.533	1.00	0.00	3A4
ATOM	1716		ASP	262	58.341	8.497 8.011	20.759 17.175	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1717 1718	C O	ASP ASP	262 262	60.828 62.015	8.125	17.477	1.00	0.00	3A4
ATOM	1719	N	THR	263	60.385	8.087	15.889	1.00	0.00	3A4
ATOM	1720	CA	THR	263	61.231	8.151	14.709	1.00	0.00	3A4
MOTA	1721	CB	THR	263	61.257	6.828	13.922	1.00	0.00	3A4
MOTA	1722		THR	263	59.962	6.247	13.768	1.00	0.00	3A4 3A4
ATOM	1723 1724	CG2	THR THR	263 263	62.163 60.819	5.831 9.346	14.677 13.857	1.00	0.00	3A4
ATOM ATOM	1725	o	THR	263	61.248	10.466	14.127	1.00	0.00	3A4
ATOM	1726	N	GLN	264	60.017	9.120	12.773	1.00	0.00	3A4
MOTA	1727	CA	GLN	264	59.831	10.032	11.649	1.00	0.00	3A4
MOTA	1728	СВ	GLN	264	59.812	9.263	10.288	1.00	0.00	3A4
ATOM	1729	CG	GLN	264 264	61.018 60.951	8.324 7.671	10.094 8.710	1.00	0.00	3A4 3A4
ATOM ATOM	1730 1731	CD OE1	GLN GLN	264	61.775	7.968	7.846	1.00	0.00	3A4
ATOM	1732		GLN	264	59.961	6.763	8.489	1.00	0.00	3A4
ATOM	1733	Ç	GLN	264	58.564	10.861	11.768	1.00	0.00	3A4
ATOM	1734	0	GLN	264	57.907	10.891	12.808	.1.00	0.00	3A4
ATOM	1735	N	LYS	265	58.214 57.091	11.556 12.459	10.645 10.453	1.00	0.00	3A4 3A4
ATOM ATOM	1736 1737	CA CB	LYS LYS	265 265	57.471	13.608	9.470	1.00	0.00	3A4
MOTA	1738	CG	LYS	265	56.414	14.703	9.209	1.00	0.00	3A4
ATOM	1739	CD	LYS	265	55.986	15.485	10.458	1.00	0.00	3A4
MOTA	1740		LYS	265	55.004	16.618	10.140	1.00	0.00	3A4
MOTA	1741	NZ	LYS	265	54.585	17.323	11.374	1.00	0.00	3A4 3A4
ATOM	1742 1743		LYS LYS	265 265	55.895 54.757	11.698 11.957	9.920 10.308	1.00	0.00	3A4
ATOM ATOM	1744	N	HIS	266	56.161	10.712	9.017			3A4
ATOM	1745		HIS	266	55.192	9.789	8.453			3A4
MOTA	1746	ND1	HIS	266	53.213	11.484	6.555			3A4
ATOM	1747		HIS	266	54.551	11.168	6.457			3A4
ATOM	1748		HIS	266	55.138 54.234	9.857 13.294	6.906 5.769			3A4 3A4
ATOM ATOM	1749 1750		HIS HIS	266 266	54.234 55.161	12.287	5.769			3A4
ATOM	1751		HIS	266	53.101	12.764	6.128			3A4
ATOM	1752		HIS	266	55.520	8.402		1.00	0.00	3A4
ATOM	1753	0	HIS	266	55.595	7.432				3A4
ATOM	1754		ARG	267	55.681	8.319				3A4 3A4
MOTA	1755		ARG		55.787 57.206	7.112 6.450				3A4
ATOM ATOM	1756 1757		ARG ARG		57.342	5.024				3A4
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ATOM	1758	CD	ARG	267	56.433	3.983	10.915	1.00	0.00	3A4
ATOM	1759	NE	ARG	267	56.515	2.666	11.644	1.00	0.00	3A4
MOTA	1760	CZ	ARG	267	55.718	2.342	12.715		0.00	3A4
ATOM	1761		ARG	267	55.829	1.104	13.280	1.00	0.00	3A4
ATOM	1762		ARG	267	54.819	3.229	13.235	1.00	0.00	3A4 3A4
ATOM	1763	C	ARG	267	55.443	7.575	12.488 12.757	1.00	0.00	3A4
ATOM	1764 1765	0	ARG VAL	267 268	55.403 55.180	8.776 6.600	13.409	1.00	0.00	3A4
ATOM ATOM	1766	N CA	VAL	268	54.850	6.700	14.830	1.00	0.00	3A4
ATOM	1767	СВ	VAL	268	55.608	7.738	15.672	1.00	0.00	3A4
ATOM	1768	CG1		268	55.286	7.564	17.181	1.00	0.00	3A4
ATOM	1769	CG2		268	57.124	7.555	15.459	1.00	0.00	3A4
MOTA	1770	С	VAL	268	53.347	6.859	14.949	1.00	0.00	3A4
ATOM	1771	0	VAL	268	52.814	7.966	14.876	1.00	0.00	3A4
MOTA	1772	N	ASP	269	52.650	5.703	15.128	1.00	0.00	3A4
ATOM	1773	CA	ASP	269	51.217	5.484	15.039	1.00	0.00	3A4
ATOM	1774	CB	ASP	269	50.952	4.008	14.629 15.562	1.00	0.00	3A4 3A4
ATOM	1775 1776	CG	ASP ASP	269 269	51.584 52.585	2.963 2.329	15.136	1.00	0.00	3A4
ATOM ATOM	1777		ASP	269	51.040	2.734	16.671	1.00	0.00	3A4
ATOM	1778	C	ASP	269	50.513	5.855	16.322	1.00	0.00	3A4
ATOM	1779	ō	ASP	269	51.163	6.144	17.324	1.00	0.00	3A4
ATOM	1780	N	PHE	270	49.161	5.834	16.331	1.00	0.00	3A4
MOTA	1781	CA	PHE	270	48.362	6.204	17.490	1.00	0.00	3A4
MOTA	1782	СВ	PHE	270	46.855	6.258	17.148	1.00	0.00	3A4
MOTA	1783	CG	PHE	270	45.990	6.766	18.282	1.00	0.00	3A4
MOTA	1784		PHE	270	45.280	5.854	19.081	1.00	0.00	3A4
ATOM	1785		PHE	270	46.020	8.114	18.661	1.00	0.00 0.00	3A4 3A4
ATOM	1786		PHE	270 270	44.531 45.309	6.282 8.546	20.177 19.789	1.00 1.00	0.00	3A4
ATOM ATOM	1787 1788	CZ	PHE	270	44.542	7.634	20.522	1.00	0.00	3A4
ATOM	1789	C	PHE	270	48.565	5.305	18.696	1.00	0.00	3A4
ATOM	1790	ŏ	PHE	270	48.623	5.789	19.822	1.00	0.00	3A4
MOTA	1791	N	LEU	271	48.707	3.980	18.488	1.00	0.00	3A4
ATOM	1792	CA	LEU	271	48.911	3.039	19.569	1.00	0.00	3A4
MOTA	1793	CB	LEU	271	48.798	1.584	19.058	1.00	0.00	3A4
MOTA	1794	CG	LEU	271	47.377	1.034	18.852	1.00	0.00	3A4
MOTA	1795		LEU	271	47.422	-0.399	18.277	1.00	0.00	3A4
ATOM	1796		LEU	271	46.550	1.035	20.150 20.287	1.00	0.00	3A4 3A4
ATOM ATOM	1797 1798	С 0	LEU LEU	271 271	50.247 50.309	3.247 3.283	21.510	1.00	0.00	3A4
ATOM	1799	N	GLN	272	51.325	3.513	19.518	1.00	0.00	3A4
ATOM	1800	CA	GLN	272	52.641	3.856	20.018	1.00	0.00	3A4
ATOM	1801	СВ	GLN	272	53.651	3.973	18.871	1.00	0.00	3A4
ATOM	1802	CG	GLN	272	53.989	2.568	18.334	1.00	0.00	3A4
MOTA	1803	CD	GLN	272	54.908	2.656	17.119	1.00	0.00	3A4
ATOM	1804		GLN	272	55.225	3.735	16.626	1.00	0.00	3A4
ATOM	1805		GLN	272	55.347	1.475	16.611	1.00	0.00	3A4
ATOM	1806	C	GLN	272	52.646	5.136 5.214	20.813	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1807 1808	O N	GLN LEU	272 273	53.254 51.883	6.155	20.356	1.00	0.00	3A4
ATOM	1809	CA	LEU	273	51.695	7.415	21.048	1.00	0.00	3A4
ATOM	1810	СB	LEU	273	50.926	8.433	20.166	1.00	0.00	3A4
ATOM	1811	CG	LEU	273	51.785	8.888	18.948	1.00	0.00	3A4
ATOM	1812	CD1	LEU	273	50.959	9.439	17.771	1.00	0.00	3A4
MOTA	1813	CD2	LEU	273	52.899	9.882	19.332	1.00	0.00	3A4
MOTA	1814	С	LEU	273	50.983	7.274	22.346	1.00	0.00	3A4
MOTA	1815	0	LEU	273	51.365	7.895	23.329	1.00	0.00	3A4
ATOM	1816	N	MET	274	49.964	6.395	22.412	1.00	0.00	3A4 3A4
ATOM	1817	CA	MET	274	49.244 47.977	6.073 5.254	23.621 23.316	1.00	0.00	3A4
ATOM ATOM	1818 1819	CB CG	MET MET	274 274	46.828	6.090	22.751	1.00	0.00	3A4
ATOM	1820	SD	MET	274	45.317	6.067	23.770	1.00	0.00	3A4
ATOM	1821	CE	MET	274	45.991	6.940	25.218	1.00	0.00	3A4
ATOM	1822	c	MET	274	50.109	5.325	24.619		0.00	3A4
ATOM	1823	0	MET	274	50.038	5.567	25.819		0.00	3A4
ATOM	1824	N	ILE	275	50.988	4.417	24.131	1.00	0.00	3A4
MOTA	1825	CA	ILE	275	51.851	3.564	24.931		0.00	3A4
MOTA	1826	CB	ILE	275	52.467	2.441	24.078		0.00	3A4 3A4
ATOM	1827		ILE	275	53.965	2.545	23.648 24.643		0.00	3A4
MOTA MOTA	1828 1829	CD	ILE ILE	275 275	52.209 51.787	1.038	23.536		0.00	3A4
A I ON	1023	CD		213	31.707	0.001				

ATOM	1830	С	ILE	275	52.925	4.329	25.660	1.00	0.00	3A4
ATOM	1831	ŏ	ILE	275	53.323	3.975	26.764	1.00	0.00	3A4
ATOM	1832	N	ASP	276	53.392	5.425	25.033	1.00	0.00	3A4
ATOM	1833	CA	ASP	276	54.488	6.233	25.491	1.00	0.00	3A4
ATOM	1834	СВ	ASP	276	55.375	6.635	24.263	1.00	0.00	3A4
ATOM	1835	CG	ASP	276	56.766	7.177	24.648	1.00	0.00	3A4
ATOM	1836	OD1	ASP	276	57.527	6.432	25.323	1.00	0.00	3A4
MOTA	1837	OD2	ASP	276	57.08 0	8.336	24.266	1.00	0.00	3A4
ATOM	1838	С	ASP	276	53.994	7.467	26.229	1.00	0.00	3A4
MOTA	1839	0	ASP	276	54.738	8.023	27.029	1.00	0.00	3A4
ATOM	1840	N	SER	277	52.734	7.918	25.959	1.00	0.00	3A4
ATOM	1841	CA	SER	277	51.962	9.005	26.574	1.00	0.00	3A4
ATOM	1842	СВ	SER	277	51.494	8.689	28.034	1.00	0.00	3A4
ATOM	1843	OG	SER	277	52.536	8.498	28.989	1.00	0.00	3A4
MOTA	1844	С	SER	277	52.586	10.401	26.477	1.00	0.00	3A4
MOTA	1845	0	SER	277	53.547	10.719	27.177	1.00	0.00	3A4
ATOM	1846	N	GLN	278	52.027	11.259	25.584	1.00	0.00	3A4
MOTA	1847	CA	GLN	278	52.576	12.557	25.230	1.00	0.00	3A4
MOTA	1848	СВ	GLN	278	53.079	12.585	23.748	1.00	0.00	3A4
ATOM	1849	CG	GLN	278	52.289	11.752	22.708	1.00	0.00	3A4
MOTA	1850	CD	GLN	278	50.896	12.317	22.436	1.00	0.00	3A4
MOTA	1851		GLN	278	49.896	11.703	22.807	1.00	0.00	3A4
ATOM	1852		GLN	278	50.821	13.500	21.767	1.00	0.00	3A4
MOTA	1853	C	GLN	278	51.568	13.647	25.534	1.00	0.00	3A4
ATOM	1854	0	GLN	278	51.306	14.524	24.712	1.00	0.00	3A4
ATOM	1855	И	ASN	279	51.016	13.632	26.775	1.00	0.00	3A4 3A4
MOTA	1856	CA	ASN	279	50.193	14.697	27.310	1.00	0.00	3A4
MOTA	1857	CB	ASN	279	48.716 47.973	14.690	26.781 27.107	1.00	0.00	3A4
ATOM	1858	CG	ASN ASN	279 279	47.305	15.999 16.089	28.136	1.00	0.00	3A4
ATOM	1859 1860		ASN	279	48.086	17.026	26.221	1.00	0.00	3A4
MOTA MOTA	1861	C	ASN	279	50.239	14.505	28.808	1.00	0.00	3A4
ATOM	1862	ŏ	ASN	279	50.626	15.409	29.546	1.00	0.00	3A4
ATOM	1863	N	SER	280	49.821	13.295	29.277	1.00	0.00	3A4
ATOM	1864	CA	SER	280	49.736	12.901	30.674	1.00	0.00	3A4
ATOM	1865	СВ	SER	280	48.334	12.330	31.056	1.00	0.00	3A4
ATOM	1866	OG	SER	280	47.313	13.268	30.740	1.00	0.00	3A4
ATOM	1867	C	SER	280	50.810	11.870	30.942	1.00	0.00	3A4
ATOM	1868	0	SER	280	51.635	11.569	30.079	1.00	0.00	3A4
ATOM	1869	N	LYS	281	50.813	11.317	32.183	1.00	0.00	3A4
MOTA	1870	CA	LYS	281	51.810	10.412	32.724	1.00	0.00	3A4
ATOM	1871	CB	LYS	281	52.318	10.863	34.135	1.00	0.00	3A4
ATOM	1872	CG	LYS	281	51.368	10.740	35.357	1.00	0.00	3A4
ATOM	1873	CD	LYS	281	50.099	11.612	35.328	1.00	0.00	3A4
MOTA	1874	CE	LYS	281	49.241	11.508	36.598	1.00	0.00	3A4
MOTA	1875	NZ	LYS	281	48.695	10.139	36.770	1.00	0.00	3A4
MOTA	1876	С	LYS	281	51.259	9.009	32.800	1.00	0.00	3A4
MOTA	1877	0	LYS	281	50.051	8.792	32.725	1.00	0.00	3A4
MOTA	1878	N	GLU	282	52.179	8.025	33.003	1.00	0.00	. 3A4
MOTA	1879	CA	GLU	282	51.902	6.623	33.252	1.00	0.00	3A4
ATOM	1880	CB	GLU	282	52.839	5.684	32.439	1.00	0.00	3A4
ATOM	1881	CG	GLU	282	54.355	5.905	32.633		0.00	3A4 3A4
ATOM	1882	CD	GLU	282	55.125	5.055	31.617	1.00	0.00	3A4
ATOM	1883		GLU	282	54.983	5.322 4.133	30.393 32.049	1.00	0.00	3A4 3A4
ATOM	1884		GLU	282 282	55.866 52.026	6.378	34.739	1.00	0.00	3A4
ATOM ATOM	1885 1886	C O	GLU GLU	282	52.842	7.002	35.416	1.00	0.00	3A4
MOTA	1887	N	THR	283	51.169	5.468	35.281	1.00	0.00	3A4
ATOM	1888	CA	THR		50.949	5.262	36.708	1.00	0.00	3A4
ATOM	1889	CB	THR		49.462	5.076	37.037	1.00	0.00	3A4
ATOM	1890		THR		48.843	4.071	36.236	1.00	0.00	3A4
ATOM	1891		THR		48.746	6.425	36.797	1.00	0.00	3A4
ATOM	1892	c	THR		51.786	4.117	37.266	1.00	0.00	3A4
ATOM	1893	ŏ	THR		51.843	3.935	38.481	1.00	0.00	3A4
ATOM	1894	N	GLU		52.457	3.329	36.385	1.00		3A4
ATOM	1895	CA	GLU		53.336	2.253	36.792			3A4
ATOM	1896	СВ	GLU		52.583	0.907	37.025			3A4
ATOM	1897	CG	GLU		53.427	-0.211	37.670		0.00	3A4
ATOM	1898	CD	GLU		52.553	-1.452	37.873			3A4
MOTA	1899	OE1	GLU	284	52.075	-2.014	36.851			3A4
MOTA	1900	OE2	GLU		52.352	-1.855	39.051			3A4
ATOM	1901	C	GLU	284	54.393	2.152	35.719	1.00	0.00	3A4

MOTA	1902	0	GLU	284	55.397	2.861	35.770	1.00	0.00	3A4
ATOM	1903	N	SER	285	54.186	1.256	34.721	1.00	0.00	3A4
MOTA	1904	CA	SER	285	55.139		33.669	1.00	0.00	3A4 3A4
ATOM	1905 1906	CB OG	SER SER	285 285	56.281 55.800	-0.008 -1.171	34.108 34.781	1.00	0.00	3A4
ATOM ATOM	1907	C	SER	285	54.331	0.438	32.510	1.00	0.00	3A4
ATOM	1908	ŏ	SER	285	54.522	-0.694	32.066	1.00	0.00	3A4
ATOM	1909	N	HIS	286	53.396	1.275	31.998	1.00	0.00	3A4
ATOM	1910	CA	HIS	286	52.522	0.926	30.901	1.00	0.00	3A4
MOTA	1911	ND1		286	49.824 50.594	1.672	32.816 32.645	1.00	0.00 0. 00	3A4 3A4
ATOM ATOM	1912 1913	CG CB	HIS HIS	286 286	51.264	0.542 0.113	31.356	1.00	0.00	3A4
ATOM	1914	NE2		286	49.782	0.592	34.753	1.00	0.00	3A4
ATOM	1915		HIS	286	50.557	-0.106	33.843	1.00	0.00	3A4
MOTA	1916	CE1	HIS	286	49.366	1.652	34.090	1.00	0.00	3A4
MOTA	1917	С	HIS	286	52.192	2.222	30.200	1.00	0.00	3A4
ATOM	1918	0	HIS	286	53.089 50.878	2.937 2.537	29.758 30.069	1.00	0.00 0.00	3A4 3A4
MOTA MOTA	1919 1920	N CA	LYS LYS	287 287	50.317	3.652	29.338	1.00	0.00	3A4
ATOM	1921	CB	LYS	287	49.136	3.180	28.453	1.00	0.00	3A4
ATOM	1922	CG	LYS	287	49.553	2.209	27.349	1.00	0.00	3A4
ATOM	1923	CĐ	LYS	287	48.717	2.529	26.095	1.00	0.00	3A4
ATOM	1924	CE	LYS	287	48.931	1.795	24.736	1.00	0.00	3A4
ATOM	1925	N2	LYS	287	47.885 49.794	2.079 4.698	23.732 30.287	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1926 1927	С 0	LYS LYS	287 287	49.794	4.548	31.504	1.00	0.00	3A4
ATOM	1928	N	ALA	288	49.185	5.771	29.701	1.00	0.00	3A4
ATOM	1929	CA	ALA	288	48.374	6.783	30.350	1.00	0.00	3A4
ATOM	1930	СВ	ALA	288	48.615	8.202	29.810	1.00	0.00	3A4
MOTA	1931	C	ALA	288	46.906	6.403	30.192	1.00	0.00	3A4 3A4
MOTA	1932 1933	O N	ALA LEU	288 289	46.333 46.245	6.618 5.810	29.125 31.226	1.00	0.00 0.00	3A4
ATOM ATOM	1933	CA	LEU	289	46.774	5.489	32.535	1.00	0.00	3A4
ATOM	1935	СВ	LEU	289	46.349	6.484	33.668	1.00	0.00	3A4
ATOM	1936	CG	LEU	289	44.839	6.740	33.920	1.00	0.00	3A4
MOTA	1937		LEU	289	44.604	7.179	35.378	1.00	0.00	3A4
ATOM	1938		LEU	289	44.221	7.776	32.951	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	1939 1940	C O	LEU LEU	289 289	46.475 46.614	4.056 3.704	32.878 34.048	1.00	0.00	3A4
ATOM	1941	N	SER	290	46.131	3.176	31.880	1.00	0.00	3A4
ATOM	1942	CA	SER	290	46.112	1.765	32.148	1.00	0.00	3A4
MOTA	1943	CB	SER	290 ·	45.026	1.325	33.179	1.00	0.00	3A4
ATOM	1944	OG	SER	290	43.728	1.835	32.895	1.00	0.00	3A4 3A4
MOTA MOTA	1945 1946	С 0	SER SER	290 290	45.931 45.432	1.008 1.483	30.867 29.847	1.00	0.00	3A4
MOTA	1947	N	ASP	291	46.293	-0.287	30.944	1.00	0.00	3A4
MOTA	1948	CA	ASP	291	46.226	-1.223	29.856	1.00	0.00	3A4
MOTA	1949	СВ	ASP	291	46.894	-2.555	30.218	1.00	0.00	3A4
MOTA	1950	CG	ASP	291	48.385	-2.331	30.513 29.555	1.00	0.00	3A4 3A4
ATOM ATOM	1951 1952		ASP	291 291	49.127 48.800	-1.982 -2.508	31.690	1.00	0.00	3A4
ATOM	1953		ASP			-1.495		1.00	0.00	3A4
ATOM	1954	0	ASP	291	44.578	-1.735	28.227	1.00	0.00	3A4
ATOM	1955		LEU	292	43.831	-1.426		1.00		3A4
MOTA	1956		LEU	292	42.433	-1.624		1.00		3A4 3A4
ATOM ATOM	1957 1958		LEU	292 292	41.659 41.910	-1.848 -3.218		1.00		3A4
ATOM	1959		LEU	292	41.502	-3.197		1.00		3A4
ATOM	1960		LEU	292	41.193	-4.362		1.00		3A4
ATOM	1961	С	LEU	292	41.827	-0.445		1.00		3A4
MOTA	1962		LEU	292	41.078	-0.602		1.00		3A4
ATOM	1963		GLU	293 293	42.216 41.794	0.784 2.025		1.00		3A4 3A4
ATOM ATOM	1964 1965		GLU GLU		42.258	3.233		1.00		3A4
ATOM	1966		GLU	293	41.403	3.396				3A4
ATOM	1967		GLU		41.950	4.520	32.046	1.00	0.00	3A4
ATOM	1968	OE:	L GLU		41.285	4.842				3A4
MOTA	1969		GLU		43.037	5.066				3A4
ATOM	1970		GLU		42.286 41.540	2.186 2.607				3A4 3A4
ATOM ATOM	1971 1972		GLU LEU		43.547	1.769				3A4
MOTA	1973		LEU		44.175	1.802				3A4
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ATOM	1974	СВ	LEU	294	45.633	1.380	26.208	1.00	0.00	3A4
MOTA	1975	CG	LEU	294	46.091	-0.086	26.051	1.00	0.00	3A4
ATOM	1976	CD1		294	46.203	-0.637	24.643	1.00	0.00	3A4
ATOM	1977	CD2		294	47.365	-0.436	26.810	1.00	0.00 0.00	3A4 3A4
ATOM	1978	C	LEU	294 294	43.443 43.172	0.944 1.361	25.134 24.020	1.00	0.00	3A4
ATOM ATOM	1979 1980	O N	LEU Val	294	43.172	-0.282	25.551	1.00	0.00	3A4
ATOM	1981	CA	VAL	295	42.358	-1.242	24.721	1.00	0.00	3A4
ATOM	1982	СВ	VAL	295	42.271	-2.600	25.380	1.00	0.00	3A4
ATOM	1983	CG1		295	41.397	-3.622	24.599	1.00	0.00	3A4
ATOM	1984	CG2	VAL	295	43.701	-3.178	25.429	1.00	0.00	3A4
ATOM	1985	С	VAL	295	40.980	-0.762	24.357	1.00	0.00	3A4
MOTA	1986	0	VAL	295	40.584	-0.846	23.207	1.00	0.00	3A4
ATOM	1987	N	ALA	296	40.252	-0.146 0.439	25.306 25.074	1.00	0.00	3A4 3A4
ATOM ATOM	1988 1989	CA CB	ALA ALA	296 296	38.945 38.344	0.902	26.408	1.00	0.00	3A4
ATOM	1990	С	ALA	296	38.944	1.619	24.132	1.00	0.00	3A4
ATOM	1991	Ö	ALA	296	38.032	1.797	23.342	1.00	0.00	3A4
ATOM	1992	N	GLN	297	40.018	2.430	24.170	1.00	0.00	3A4
MOTA	1993	CA	GLN	297	40.228	3.546	23.284	1.00	0.00	3A4
ATOM	1994	СВ	GLN	297	41.379	4.436	23.773	1.00	0.00	3A4
MOTA	1995	CG	GLN	297	40.914	5.233	25.008	1.00	0.00	3A4
MOTA	1996	CD	GLN	297	42.099	5.887	25.715	1.00	0.00	3A4 3A4
ATOM	1997		GLN	297 297	43.052 42.034	5.222 7.228	26.114 25.902	1.00	0.00	3A4
ATOM ATOM	1998 1999	C	GLN GLN	297	40.505	3.108	21.882	1.00	0.00	3A4
ATOM	2000	Ö	GLN	297	39.872	3.572	20.943	1.00	0.00	3A4
ATOM	2001	N	SER	298	41.403	2.117	21.715	1.00	0.00	3A4
ATOM	2002	CA	SER	298	41.744	1.546	20.434	1.00	0.00	3A4
MOTA	2003	CB	SER	298	42.925	0.563	20.529	1.00	0.00	3A4
MOTA	2004	OG	SER	298	42.771	-0.519	21.435	1.00	0.00	3A4
ATOM	2005	c	SER	298	40.584	0.872	19.755	1.00	0.00	3A4 3A4
ATOM ATOM	2006 2007	O N	SER ILE	298 299	40.435 39.688	0.977 0.228	18.546 20.542	1.00	0.00	3A4
ATOM	2007	CA	ILE	299	38.438	-0.363	20.098	1.00	0.00	3A4
ATOM	2009	СВ	ILE	299	37.670	-1.032	21.291	1.00	0.00	3A4
ATOM	2010		ILE	299	36.134	-1.268	21.098	1.00	0.00	3A4
MOTA	2011	CG1	ILE	299	38.328	-2.333	21.803	1.00	0.00	3A4
MOTA	2012	CD	ILE	299	37.787	-3.619	21.185	1.00	0.00	3A4
MOTA	2013	С	ILE	299	37.515	0.677	19.534	1.00	0.00	3A4
ATOM	2014	O N	ILE	299 300	36.949 37.374	0.525 1.799	18.457 20.268	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2015 2016	CA	ILE	300	36.494	2.883	19.921	1.00	0.00	3A4
ATOM	2017	СВ	ILE	300	36.290	3.798	21.113	1.00	0.00	3A4
ATOM	2018		ILE	300	36.292	5.340	20.897	1.00	0.00	3A4
ATOM	2019	CG1	ILE	300	34.906	3.296	21.637	1.00	0.00	3A4
MOTA	2020	CD	ILE	300	34.503	3.642	23.050	1.00	0.00	3A4
ATOM	2021	C	ILE	300	36.962	3.618 3.994	18.712	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2022 2023	O N	ILE PHE	300 3 01	36.161 38.279	3.774	17.872 18.515	1.00	0.00	3A4
ATOM	2024	CA	PHE	301	38.819	4.525	17.406	1.00	0.00	3A4
ATOM	2025	CB	PHE	301	40.332	4.745		1.00	0.00	3A4
ATOM	2026	CG	PHE	301	40.520	5.958	18.535	1.00	0.00	3A4
ATOM	2027		PHE	301	41.157	5.931		1.00	0.00	3A4
MOTA	2028		PHE	301	39.913	7.144	18.106	1.00	0.00	3A4
ATOM	2029 2030		PHE	301 301	41.032 39.784	7.015 8.213		1.00	0.00	3A4 3A4
MOTA MOTA	2030	CZ	PHE	301	40.300	8.142		1.00	0.00	3A4
ATOM	2032	ç	PHE	301	38.633	3.743		1.00	0.00	3A4
ATOM	2033	Ó	PHE	301	38.332	4.306		1.00	0.00	3A4
ATOM	2034	N	ILE	302	38.742	2.401	16.178	1.00	0.00	3A4
MOTA	2035	CA	ILE	302	38.511	1.491				3A4
ATOM	2036	CB	ILE	302	39.005	0.104		1.00		3A4
ATOM	2037		ILE	302	38.482	-1.056				3A4 3A4
MOTA MOTA	2038 2039	CD	ILE	302 302	40.563 41.293	0.105 0.195				3A4
MOTA	2039	C	ILE		37.054	1.462				3A4
ATOM	2041	ŏ	ILE	302	36.732	1.682				3A4
ATOM	2042	N	PHE	303	36.126	1.231	15.610	1.00		3A4
MOTA	2043	CA	PHE		34.711	1.090				3A4
MOTA	2044	СВ	PHE		34.008	0.159				3A4
ATOM	2045	CG	PHE	303	33.072	0.735	17.449	1.00	0.00	3A4

ATOM	2046	CD1	PHE	303	31.783	1.209	17.127	1.00	0.00	3A4
ATOM	2047	CD2		303	33.443	0.706	18.808	1.00	0.00	3A4
MOTA	2048	CE1		303	30.911	1.674	18.121	1.00	0.00	3A4 3A4
ATOM	2049	CE2		303	32.572	1.155 1.647	19.810 19.465	1.00	0.00	3A4
ATOM ATOM	2050 2051	CZ C	PHE	303 303	31.307 34.016	2.407	14.993	1.00	0.00	3A4
ATOM	2052	ŏ	PHE	303	33.183	2.472	14.092	1.00	0.00	3A4
ATOM	2053	N	ALA	304	34.391	3.513	15.679	1.00	0.00	3A4
MOTA	2054	CA	ALA	304	33.814	4.831	15.484	1.00	0.00	3A4
MOTA	2055	СВ	ALA	304	34.124	5.826	16.638	1.00	0.00	3A4 3A4
ATOM	2056	C	ALA	304 304	34.221 33.449	5.470 6.196	14.208 13.589	1.00	0.00	3A4
ATOM ATOM	2057 2058	о И	ALA GLY	305	35.466	5.191	13.787	1.00	0.00	3A4
ATOM	2059	CA	GLY	305	36.037	5.755	12.599	1.00	0.00	3A4
ATOM	2060	C	GLY	305	35.766	5.044	11.304	1.00	0.00	3A4
MOTA	2061	0	GLY	305	36.028	5.603	10.243	1.00	0.00	3A4
MOTA	2062	N	TYR	306	35.257	3.789	11.337	1.00	0.00	3A4 3A4
ATOM	2063	CA	TYR TYR	306 306	35.125 35.531	2.982 1.484	10.139	1.00	0.00 0.00	3A4
MOTA MOTA	2064 2065	CB CG	TYR	306	35.403	0.528	9.206	1.00	0.00	3A4
ATOM	2066		TYR	306	35.378	0.950	7.858	1.00	0.00	3A4
ATOM	2067		TYR	306	35.195	-0.835	9.469	1.00	0.00	3A4
MOTA	2068		TYR	306	35.009	0.064	6.843	1.00	0.00	3A4
MOTA	2069		TYR	306	34.885	-1.738	8.441	1.00	0.00	3A4 3A4
ATOM	2070	CZ	TYR	306 306	34.766 34.383	-1.281 -2.159	7.125 6.089	1.00	0.00 0.00	3A4
ATOM ATOM	2071 2072	OH C	TYR TYR	306	33.741	3.132	9.572	1.00	0.00	3A4
ATOM	2073	ŏ	TYR	306	33.566	3.553	8.431	1.00	0.00	3A4
ATOM	2074	N	GLU	307	32.692	2.781	10.344	1.00	0.00	3A4
MOTA	2075	CA	GLU	307	31.384	2.639	9.745	1.00	0.00	3A4
ATOM	2076	CB	GLU	307	30.517	1.553	10.437 10.329	1.00	0.00	3A4 3A4
ATOM ATOM	2077 2078	CG CD	GLU GLU	307 307	31.119 31.130	0.127 -0.460	8.905	1.00	0.00	3A4
ATOM	2079		GLU	307	30.600	0.159	7.942	1.00	0.00	3A4
ATOM	2080		GLU	307	31.670	-1.592	8.778	1.00	0.00	3A4
ATOM	2081	С	GLU	307	30.630	3.933	9.563	1.00	0.00	3A4
MOTA	2082	0	GLU	307	29.605	3.926	8.924	1.00	0.00	3A4
ATOM	2083	N	THR	308	31.140	5.089 6.394	10.026 9.788	1.00	0.00	3A4 3A4
MOTA MOTA	2084 2085	CA CB	THR THR	308 308	30.556 30.866	7.363	10.932	1.00	0.00	3A4
ATOM	2086		THR	308	32.255	7.423	11.254	1.00	0.00	3A4
ATOM	2087		THR	308	30.088	6.935	12.191	1.00	0.00	3A4
MOTA	2088	С	THR	308	31.006	6.957	8.463	1.00	0.00	3A4
ATOM	2089	0	THR	308	30.202	7.360	7.632 8.226	1.00	0.00	3A4 3A4
ATOM ATOM	2090 2091	N CA	THR	309 309	32.332 32.979	6.929 7.436	7.038	1.00	0.00	3A4
ATOM	2092	CB	THR	309	34.479	7.445	7.204	1.00	0.00	3A4
ATOM	2093	OG1		309	34.937	6.213	7.743	1.00	0.00	3A4
MOTA	2094	CG2		309	34.867	8.555	8.200	1.00	0.00	3A.4
ATOM	2095	C	THR	309	32.600	6.684	5.779	1.00	0.00	3A4 3A4
ATOM	2096 2097	0 N	THR	309 310	32.349 32.484	7.278 5.339	4.741 5.875	1.00	0.00	3A4
ATOM	2098	N CA	SER SER	310	32.052	4.458	4.809	1.00	0.00	3A4
ATOM	2099	СВ	SER	310	31.996	2.990	5.310	1.00	0.00	3A4
MOTA	2100	OG	SER	310	33.306	2.563	5.646		0.00	3A4
MOTA	2101	C	SER	310	30.666	4.763	4.322	1.00	0.00	3A4
ATOM	2102	0	SER	310	30.413	4.886	3.131	1.00	0.00	3A4 3A4
ATOM ATOM	2103 2104	N CA	SER SER	311 311	29.728 28.351	4.960 5.245	5.261 4.950		0.00	3A4
ATOM	2105	CB	SER		27.509	5.056	6.222		0.00	3A4
ATOM	2106	ŌĞ	SER		27.701	3.739	6.719	1.00	0.00	3A4
ATOM	2107	С	SER		28.153	6.627	4.389			3A4
ATOM	2108	0	SER		27.316	6.833	3.523			3A4
ATOM	2109 2110	N	VAL	312 312	28.984 28.964	7.609 8.970	4.813 4.310			3A4 3A4
MOTA MOTA	2110	CA CB	VAL VAL		28.964	9.902	5.173			3A4
ATOM	2112		VAL		29.980	11.315	4.570			3A4
ATOM	2113		VAL		28.894	10.077	6.433			3A4
MOTA	2114	C	VAL		29.408	9.072	2.884			3A4
ATOM	2115	0	VAL		28.751	9.739				3A4 3A4
ATOM	2116		LEU		30.463 30.996	8.328 8.277				3A4
ATOM	2117	CH	PEV	213	30.220	9.211	1.150	1.00	5.00	5.11

MOTA	2118	СВ	LEU	313	32.294	7.466	1.085	1.00	0.00	3A4
MOTA	2119		LEU	313	33.512	8.219	1.649	1.00	0.00	3A4
ATOM	2120	CD1		313	34.492	8.511	0.499	1.00	0.00	3A4 3A4
ATOM ATOM	2121 2122	CD2 C	LEU	313 313	33.322 30.017	9.485 7.696	2.496 0.167	1.00	0.00	3A4
ATOM	2123	o	LEU	313	29.808	8.229	-0.917	1.00	0.00	3A4
ATOM	2124	N	SER	314	29.309	6.624	0.579	1.00	0.00	3A4
MOTA	2125	CA	SER	314	28.305	5.981	-0.243	1.00	0.00	3A4
MOTA	2126	CB	SER	314	27.992	4.570	0.299	1.00	0.00	3A4
MOTA	2127	OG	SER	314	29.195	3.821	0.397	1.00	0.00	3A4
ATOM	2128	C	SER	314	27.070 26.505	6.845 6.909	-0.420 -1.507	1.00	0.00	3A4 3A4
ATOM ATOM	2129 2130	O N	SER	314 315	26.702	7.636	0.625	1.00	0.00	3A4
ATOM	2131	CA	PHE	315	25.595	8.572	0.583	1.00	0.00	3A4
ATOM	2132	СВ	PHE	315	25.181	9.076	2.015	1.00	0.00	3A4
MOTA	2133	CG	PHE	315	23.897	8.407	2.456	1.00	0.00	3A4
ATOM	2134	CD1		315	23.856	7.678	3.662	1.00	0.00	3A4
ATOM	2135	CD2		315	22.732	8.451 7.024	1.660 4.067	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2136 2137		PHE	315 315	22.683 21.568	7.770	2.047	1.00	0.00	3A4
ATOM	2138	CZ	PHE	315	21.542	7.061	3.254	1.00	0.00	3A4
ATOM	2139	C	PHE	315	25.938	9.760	-0.291	1.00	0.00	3A4
ATOM	2140	0	PHE	315	25.075	10.250	-1.011	1.00	0.00	3A4
ATOM	2141	N	ILE	316	27.230	10.200	-0.328	1.00	0.00	3A4
MOTA	2142	CA	ILE	316	27.669	11.286	-1.202	1.00	0.00	3A4 3A4
ATOM ATOM	2143 2144	CB	ILE ILE	316 316	29.119 29.128	11.864 13.291	-1.060 -1.688	1.00	0.00 0.00	3A4
ATOM	2145		ILE	316	29.687	11.833	0.371	1.00	0.00	3A4
ATOM	2146	CD	ILE	316	30.950	12.629	0.687	1.00	0.00	3A4
MOTA	2147	С	ILE	316	27.559	10.926	-2.666	1.00	0.00	3A4
ATOM	2148	0	ILE	316	27.111	11.726	-3.476	1.00	0.00	3A4
ATOM	2149	N	MET	317	27.919	9.671	-3.009	1.00	0.00	3A4 3A4
ATOM ATOM	2150 2151	CA CB	MET MET	317 317	27.868 28.640	9.137 7.803	-4.351 -4.441	1.00	0.00 0.00	3A4
ATOM	2152	CG	MET	317	30.148	8.007	-4.191	1.00	0.00	3A4
ATOM	2153	SD	MET	317	31.027	6.548	-3.550	1.00	0.00	3A4
ATOM	2154	CE	MET	317	32.475	7.489	-2.987	1.00	0.00	3A4
ATOM	2155	С	MET	317	26.449	8.978	-4.853	1.00	0.00	3A4
ATOM	2156	0	MET	317	26.139	9.327	-5.986	1.00	0.00	3A4 3A4
MOTA MOTA	2157 2158	N CA	TYR TYR	318 318	25.516 24.101	8.539 8.458	-3.981 -4.293	1.00	0.00	3A4
ATOM	2159	CB	TYR	318	23.333	7.794	-3.134	1.00	0.00	3A4
ATOM	2160	CG	TYR	318	21.822	7.683	-3.312	1.00	0.00	3A4
MOTA	2161	CD1	TYR	318	21.269	7.039	-4.436	1.00	0.00	3A4
MOTA	2162		TYR	318	. 20.950	8.269	-2.372	1.00	0.00	3A4
ATOM	2163		TYR	318	19.881	6.987 8.209	-4.624 -2.548	1.00	0.00	3A4 3A4
ATOM ATOM	21.64 2165	CZ	TYR TYR	318 318	19.560 19.024	7.566	-3.675	1.00	0.00	3A4
MOTA	2166	ОН	TYR	318	17.625	7.498	-3.855	1.00	0.00	. 3A4
ATOM	2167	С	TYR	318	23.501	9.814	-4.592	1.00	0.00	3A4
MOTA	2168	0	TYR	318	22.759	9.967	-5.553	1.00	0.00	3A4
ATOM	2169	И	GLU		23.864	10.847	-3.796	1.00	0.00	3A4 3A4
ATOM ATOM	2170 2171	CA CB	GLU GLU	319 319	23.389 23.703	12.203 13.127	-3.970 -2.775	1.00	0.00	3A4
ATOM	2172	CG	GLU	319	22.849	12.760	-1.559	1.00	0.00	3A4
ATOM	2173	CD	GLU	319	23.038	13.838	-0.506	1.00	0.00	3A4
ATOM	2174		GLU	319	24.202	14.049	-0.085	1.00	0.00	3A4
ATOM	2175		GLU	319	22.027	14.476	-0.119	1.00	0.00	3A4
ATOM	2176	C	GLU	319	23.894	12.847	-5.231	1.00	0.00	3A4 3A4
MOTA MOTA	2177 2178	O N	GLU LEU	319 320	23.132 25.170	13.474 12.641	-5.951 -5.595	1.00	0.00	3A4
MOTA	2179	CA	LEU		25.713	13.161	-6.828	1.00	0.00	3A4
ATOM	2180	СВ	LEU		27.239	13.059	-6.841	1.00	0.00	3A4
ATOM	2181	CG	LEU	320	27.880	14.027	-5.843	1.00	0.00	3A4
MOTA	2182		LEU		29.380	13.757	-5.709	1.00	0.00	3A4
MOTA	2183		LEU		27.611	15.489	-6.192	1.00	0.00	3A4
ATOM	2184	C O	LEU		25.160 24.977	12.475 13.105	-8.048 -9.083	1.00	0.00	3A4 3A4
MOTA MOTA	2185 2186	N	LEU ALA		24.818	11.177	-7.933		0.00	3A4
MOTA	2187	CA	ALA		24.215	10.397	-8.990			3A4
ATOM	2188	СВ	ALA	321	24.217	8.897	-8.645	1.00	0.00	3A4
ATOM	2189	С	ALA		22.802	10.861	-9.259	1.00	0.00	3A4

МОТА	2190	0	ALA	321	22.338	10.884	-10.397		0.00	3A4
MOTA	2191	N	THR	322		11.305	-8.194		0.00	3A4
ATOM	2192	CA	THR	322		11.780	-8.258		0.00 0.00	3A4 3A4
ATOM	2193	CB OG1	THR	322 322		11.519 11.999	-6.972 -5.794	1.00	0.00	3A4
ATOM ATOM	2194 2195	CG2		322	19.745	9.994	-6.849	1.00	0.00	3A4
ATOM	2196	C	THR	322		13.242	-8.642	1.00	0.00	3A4
ATOM	2197	0	THR	322	19.555	13.704	-9.018	1.00	0.00	3A4
MOTA	2198	N	HIS	323	21.731	14.006	-8.558	1.00	0.00	3A4
ATOM	2199	CA	HIS	323	21.740	15.416	-8.856 -5.650	1.00	0.00	3A4 3A4
ATOM ATOM	2200 2201	ND1 CG	HIS	323 323	20.544 20.676	15.212 16.147	-6.653	1.00	0.00	3A4
ATOM	2202	СВ	HIS	323	21.859	16.259	-7.581	1.00	0.00	3A4
ATOM	2203	NE2		323	18.715	16.470	-5.582	1.00	0.00	3A4
ATOM	2204	CD2		323	19.549	16.908	-6.595	1.00	0.00	3A4
ATOM	2205	CE1		323	19.356	15.449	-5.043 -9.775	1.00	0.00	3A4 3A4
ATOM	2206	C	HIS HIS	323 323	22.892 23.883	15.711 16.309	-9.352	1.00	0.00	3A4
ATOM ATOM	2207 2208	O N	PRO	324	22.833		-11.076	1.00	0.00	3A4
ATOM	2209	CA	PRO	324	23.958		-12.002	1.00	0.00	3A4
MOTA	2210	CD	PRO	324	21.602		-11.765	1.00	0.00	3A4
MOTA	2211	СВ	PRO	324	23.420		-13.300	1.00	0.00	3A4 3A4
MOTA	2212	CG	PRO	324	21.905 24.415		-13.255 -12.213	1.00	0.00	3A4
ATOM ATOM	2213 2214	С О	PRO PRO	324 324	25.575		-12.534	1.00	0.00	3A4
ATOM	2215	N	ASP	325	23.561		-11.949	1.00	0.00	3A4
MOTA	2216	CA	ASP	325	23.917		-12.002	1.00	0.00	3A4
ATOM	2217	CB	ASP	325	22.668		-11.821	1.00	0.00	3A4 3A4
ATOM	2218	CG	ASP	325	21.653 21.991		-12.931 -14.125	1.00	0.00 0.00	3A4
ATOM ATOM	2219 2220		ASP ASP	325 325	20.531		-12.600	1.00	0.00	3A4
ATOM	2221	C	ASP	325	24.927		-10.944	1.00	0.00	3A4
ATOM	2222	0	ASP	325	25.817		-11.169	1.00	0.00	3A4
MOTA	2223	N	VAL	326	24.835	19.071	-9.767	1.00	0.00	3A4 3A4
ATOM	2224	CA	VAL	326	25.742 25.198	19.249 18.672	-8.647 -7.341	1.00	0.00 0.00	3A4
ATOM ATOM	2225 2226	·CB	VAL VAL	326 326	26.201	18.872	-6.173	1.00	0.00	3A4
ATOM	2227		VAL	326	23.874	19.402	-7.034	1.00	0.00	3A4
MOTA	2228	С	VAL	326	27.083	18.648	-8.960	1.00	0.00	3A4
MOTA	2229	0	VAL	326	28.106	19.288	-8.782	1.00	0.00	3A4 3A4
ATOM ATOM	2230 2231	N CA	GLN GLN	327 327	27.089 28.281	17.427 16.718	-9.528 -9.931	1.00	0.00	3A4
ATOM	2232	СВ	GLN	327	27.899		-10.487	1.00	0.00	3A4
ATOM	2233	CG	GLN	327	29.062	14.350	-10.683	1.00	0.00	3A4
MOTA	2234	CD	GLN	327	28.538		-11.166	1.00	0.00	3A4
ATOM	2235		GLN	327	27.336 29.475		-11.186 -11.572	1.00	0.00	3A4 3A4
ATOM ATOM	2236 2237	C NEZ	GLN GLN	327 327	29.088		-10.960	1.00	0.00	3A4
ATOM	2238	ŏ	GLN	327	30.301		-10.855	1.00	0.00	3A4
ATOM	2239	N	GLN	328	28.408		-11.941	1.00	0.00	3A4
ATOM	2240	CA	GLN	328	29.023		-12.995	1.00	0.00	3A4 3A4
ATOM	2241 2242	CB	GLN GLN	328 328	27.977 27.544		-14.041 -14.957	1.00	0.00	3A4
ATOM ATOM	2243	CD	GLN	328	26.423		-15.885	1.00	0.00	3A4
ATOM	2244		GLN	328	26.675	19.426	-16.800		0.00	3A4
MOTA	2245		GLN	328	25.164		-15.654	1.00	0.00	3A4
MOTA	2246		GLN	328	29.711		-12.470	1.00	0.00	3A4 3A4
ATOM ATOM	2247 2248	O N	GLN LYS	328 329	30.827 29.068		-12.855 -11.501	1.00		3A4
ATOM	2249		LYS	329	29.597		-10.807			3A4
ATOM	2250		LYS	329	28.515	22.465				3A4
MOTA	2251	CG	LYS	329	28.752	23.857				3A4
ATOM	2252		LYS	329	27.533	24.347 25.785				3A4 3A4
ATOM ATOM	2253 2254		LYS LYS	329 329	27.679 26.477	26.210				3A4
ATOM	2255		LYS		30.884		-10.052			3A4
ATOM	2256		LYS	329	31.860		-10.101			3A4
MOTA	2257		LEU		30.952	20.423				3A4 3A4
ATOM	2258		LEU LEU		32.100 31.814	19.968 18.742				3A4
ATOM ATOM	2259 2260		LEU		30.502	18.756				3A4
ATOM	2261		1 LEU		30.541	17.732				3A4

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ATOM	2262	CD2	LEU	330	29.986	20.145	-6.584	1.00	0.00	3A4
MOTA	2263	С	LEU	330	33.250	19.598	-9.579	1.00	0.00	3A4
ATOM	2264	0	LEU	330	34.410	19.864	-9.296	1.00	0.00	3A4
ATOM ATOM	2265	N	GLN	331 331	32.931 33.881	18.993 18.627		1.00	0.00	3A4 3A4
ATOM	2266 2267	CA CB	GLN GLN	331	33.229	17.787		1.00	0.00	3A4
ATOM	2268	CG	GLN	331	32.942	16.354		1.00	0.00	3A4
ATOM	2269	CD	GLN	331	32.147		-13.437	1.00	0.00	3A4
ATOM	2270	OE1	GLN	331	31.063	15.988	-13.839	1.00	0.00	3A4
ATOM	2271	NE2	GLN	331	32.677		-13.885	1.00	0.00	3A4
ATOM	2272	C	GLN	331	34.500		-12.447	1.00	0.00	3A4 3A4
ATOM ATOM	2273 2274	O N	GLN GLU	331 332	35.682 33.723		-12.771 -12.594	1.00	0.00	3A4 3A4
ATOM	2275	CA	GLU	332	34.188		-13.099	1.00	0.00	3A4
ATOM	2276	СВ	GLU	332	33.019		-13.413	1.00	0.00	3A4
MOTA	2277	CG	GLU	332	32.212	22.808	-14.675	1.00	0.00	3A4
ATOM	2278	CD	GLU	332	33.080		-15.931	1.00	0.00	3A4
ATOM	2279		GLU	332	33.533		-16.217	1.00	0.00	3A4 3A4
ATOM	2280 2281		GTN GTN	332 332	33.301 35.190		-16.622 -12.182	1.00	0.00 0.00	3A4
ATOM ATOM	2282	c o	GLU	332	35.834		-12.629	1.00	0.00	3A4
ATOM	2283	N	GLU	333	35.484		-10.947	1.00	0.00	3A4
MOTA	2284	CA	GLU	333	36.662	22.661	-10.132	1.00	0.00	3A4
ATOM	2285	СВ	GLU	333	36.449	22.284	-8.639	1.00	0.00	3A4
ATOM	2286	CG	GLU	333	35.228	22.936	-7.985	1.00	0.00	3A4
ATOM	2287	CD	GLU	333	35.046	22.273	-6.620	1.00	0.00	3A4 3A4
ATOM ATOM	2288 2289		GLU GLU	333 333	35.918 34.038	22.455 21.540	-5.730 -6.462	1.00	0.00	3A4
ATOM	2290	C	GLU	333	37.923		-10.581	1.00	0.00	3A4
ATOM	2291	ō	GLU	333	38.425	21.038	-9.874	1.00	0.00	3A4
MOTA	2292	N	ILE	334	38.469	22.262	-11.773	1.00	0.00	3A4
ATOM	2293	CA	ILE	334	39.710		-12.300	1.00	0.00	3A4
MOTA	2294	CB	ILE	334	39.559		-12.973	1.00	0.00	3A4
MOTA	2295	CG2 CG1		334 334	38.582 40.932		-14.182 -13.257	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2296 2297	CD	ILE	334	40.838		-13.257	1.00	0.00	3A4
ATOM	2298	c	ILE	334	40.231		-13.189	1.00	0.00	3A4
ATOM	2299	o	ILE	334	40.570		-14.358	1.00	0.00	. 3A4
ATOM	2300	N	ASP	335	40.294		-12.600	1.00	0.00	3A4
ATOM	2301	CA	ASP	335	40.593		-13.260	1.00	0.00	3A4
ATOM	2302	CB	ASP	335	39.726		-12.699 -12.943	1.00	0.00	3A4 3A4
ATOM ATOM	2303 2304	CG OD1	ASP ASP	335 335	38.240 37.854		-14.129	1.00	0.00	3A4
ATOM	2305	OD2		335	37.469		-11.947	1.00	0.00	3A4
ATOM	2306	С	ASP	335	42.054		-13.079	1.00	0.00	3A4
MOTA	2307	0	ASP	335	42.537		-11.956	1.00	0.00	3A4
ATOM	2308	N	ALA	336	42.772		-14.223	1.00	0.00	3A4
ATOM	2309	CA CB	ALA	336	44.168 45.027		-14.316 -15.028	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2310 2311	СВ	ALA ALA	336 336	44.207		-15.025	1.00	0.00	3A4
ATOM	2312	ŏ	ALA	336	44.428		-16.275	1.00	0.00	3A4
MOTA	2313	N	VAL	337	43.963	28.609	-14.313	1.00	0.00	3A4
ATOM	2314	CA	VAL	337	43.815		-14.773	1.00	0.00	3A4
MOTA	2315	CB	VAL	337	42.641		-14.085	1.00		3A4
ATOM	2316		VAL	337	42.436		-14.612 -14.326	1.00	0.00	3A4 3A4
ATOM ATOM	2317 2318	C	VAL VAL	337 337	41.367 45.115		-14.492	1.00		3A4
ATOM	2319	ŏ	VAL	337	45.661		-13.394	1.00		3A4
ATOM	2320	N	LEU	338	45.621		-15.517	1.00		3A4
ATOM	2321	CA	LEU	338	46.821	32.257	-15.500	1.00		3A4
ATOM	2322	СВ	LEU	338	47.678		-16.799	1.00		3A4
ATOM	2323	CG	LEU	338	48.507		-16.897	1.00		3A4
ATOM ATOM	2324 2325		LEU LEU	338 338	47.680 49.592		-17.124 -17.984	1.00		3A4 3A4
ATOM	2325	CD2	LEU	338	46.355		-15.361	1.00		3A4
ATOM	2327	ŏ	LEU	338	45.265		-15.844	1.00		3A4
ATOM	2328	N	PRO	339	47.103		-14.719			3A4
ATOM	2329	CA	PRO	339	46.612		-14.286			3A4
ATOM	2330	CD	PRO		48.443		-14.196			3A4
ATOM	2331	CB	PRO	339 339	47.610 48.922		5 -13.189 9 -13.552			3A4 3A4
ATOM ATOM	2332 2333	CG	PRO PRO		48.922		-15.332 -15.437			3A4
		-							-	

ATOM	2334	0	PRO	339	47.465	36.980	-16.272	1.00	0.00	3A4
MOTA	2335	N	ASN	340	45.491	37.790		1.00	0.00	3A4
MOTA	2336	CA	ASN	340	45.246	38.810		1.00	0.00	3A4
ATOM	2337	CB	ASN	340	44.189	38.343		1.00	0.00	3A4 3A4
ATOM ATOM	2338 2339	CG OD1	ASN	340 340	44.036 42.986	39.320 39.942		1.00	0.00	3A4
ATOM	2340	ND2		340	45.094	39.457		1.00	0.00	3A4
ATOM	2341	C	ASN	340	44.785	40.012		1.00	0.00	3A4
MOTA	2342	0	ASN	340	45.452	41.045	-15.645	1.00	0.00	3A4
ATOM	2343	N	LYS	341	43.617		-14.997	1.00	0.00	3A4
ATOM	2344	CA	LYS	341	43.059		-14.095	1.00	0.00	3A4 3A4
ATOM ATOM	2345 2346	CB CG	LYS	341 341	42.250 41.892		-14.822 -13.936	1.00	0.00	3A4
ATOM	2347	CD	LYS	341	41.220		-14.664	1.00	0.00	3A4
ATOM	2348	CE	LYS	341	39.708		-14.924	1.00	0.00	3A4
ATOM	2349	NZ	LYS	341	39.409		-15.994	1.00	0.00	3A4
ATOM	2350	С	LYS	341	42.197		-13.158	1.00	0.00	3A4
ATOM	2351	0	LYS	341	40.991		-13.036	1.00	0.00	3A4
ATOM	2352	N	ALA	342	42.834		-12.482 -11.577	1.00	0.00	3A4 3A4
ATOM ATOM	2353 2354	CA CB	ALA ALA	342 342	42.189 41.316		-12.306	1.00	0.00	3A4
ATOM	2355	C	ALA	342	43.313		-10.839	1.00	0.00	3A4
ATOM	2356	ō	ALA	342	44.413		-11.386	1.00	0.00	3A4
MOTA	2357	N	PRO	343	43.106	36.880	-9.614	1.00	0.00	3A4
MOTA	2358	CA	PRO	343	44.072	36.050	-8.891	1.00	0.00	3A4
ATOM	2359	CD	PRO	343	41.953	37.220	-8.779	1.00	0.00	3A4
ATOM	2360	CB CG	PRO	343	43.605 42.097	36.121 36.392	-7.421 -7.496	1.00	0.00	3A4 3A4
ATOM ATOM	2361 2362	C	PRO PRO	343 343	44.071	34.607	-9.441	1.00	0.00	3A4
ATOM.	2363	ŏ	PRO	343	42.970	34.083	-9.619	1.00	0.00	3A4
ATOM	2364	N	PRO	344	45.209	33.930	-9.727	1.00	0.00	3A4
ATOM	2365	CA	PRO	344	45.259	32.659	-10.448	1.00	0.00	3A4
ATOM	2366	CD	PRO	344	46.542	34.509	-9.559	1.00	0.00	3A4
ATOM	2367	CB	PRO	344	46.678		-11.047	1.00	0.00	3A4
ATOM	2368	CG	PRO	344	47.532	33.459	-10.077 -9.520	1.00	0.00	3A4 3A4
ATOM ATOM	2369 2370	С 0	PRO PRO	344 344	45.002 45.522	31.443	-8.404	1.00	0.00	3A4
ATOM	2371	N	THR	345	44.206		-10.004	1.00	0.00	3A4
ATOM	2372	CA	THR	345	43.860	29.247	-9.324	1.00	0.00	3A4
ATOM	2373	CB	THR	345	42.343	29.124	-9.107	1.00	0.00	3A4
ATOM	2374		THR	345	41.981	27.994	-8.315	1.00	0.00	3A4
ATOM	2375		THR	345	41.532		-10.430	1.00	0.00	3A4 3A4
ATOM ATOM	2376 2377	С 0	THR THR	345 345	44.457 44.489		-10.173 -11.397	1.00	0.00	3A4
ATOM	2378	N	TYR	346	44.964	27.063	-9.521	1.00	0.00	3A4
ATOM	2379	CA	TYR	346	45.601		-10.173	1.00	0.00	3A4
ATOM	2380	CB	TYR	346	47.162	25.970	-10.121	1.00	0.00	3A4
MOTA	2381	CG	TYR	346	47.679		-10.925	1.00	0.00	3A4
ATOM	2382		TYR	346	48.250		-10.287	1.00	0.00	3A4
ATOM ATOM	2383 2384		TYR TYR	346 346	47.581 48.713		-12.331 -11.032	1.00	0.00	3A4 3A4
ATOM	2385		TYR	346	48.037		-13.082	1.00	0.00	3A4
ATOM	2386	CZ	TYR	346	48.606		-12.431	1.00	0.00	3A4
ATOM	2387	OH	TYR	346	49.065	30.442	-13.178	1.00	0.00	3A4
ATOM	2388	С	TYR	346	45.106	24.709		1.00	0.00	3A4
ATOM	2389	0	TYR	346	45.423	24.491		1.00	0.00	3A4
ATOM	2390	N	ASP	347	44.302		-10.168 -9.683	1.00 1.00	0.00	3A4 3A4
MOTA MOTA	2391 2392	CA CB	ASP ASP	347 347	43.715 42.187	22.647 22.761		1.00	0.00	3A4 3A4
ATOM	2393	CG	ASP	347	41.948	23.760			0.00	3A4
ATOM	2394		ASP	347	41.329	24.825			0.00	3A4
ATOM	2395		ASP	347	42.386	23.474			0.00	3A4
ATOM	2396	С	ASP	347	43.937		-10.781	1.00	0.00	3A4
ATOM	2397	0	ASP	347	43.549		-11.927		0.00	3A4
ATOM	2398 2399	N Ca	THR	348 348	44.581 44.908		-10.427 -11.314		0.00	3A4 3A4
ATOM ATOM	2399	CA CB	THR THR	348 348	46.416		-11.501		0.00	3A4
ATOM	2401		THR	348	46.987		-12.006		0.00	3A4
ATOM	2402		THR	348	46.725		-12.500		0.00	3A4
ATOM	2403	С	THR		44.258		-10.688		0.00	3A4
ATOM	2404	0	THR	348	43.393		-11.293		0.00	3A4
ATOM	2405	N	VAL	349	44.670	17.854	-9.434	1.00	0.00	3A4

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ATOM	2406	CA	VAL	349	44.059	16.848	-8.590	1.00	0.00	3A4
ATOM	2407	СВ	VAL	349	44.630	15.437	-8.788	1.00	0.00	3A4
MOTA	2408	CG1	VAL	349	46.169	15.347	-8.617	1.00	0.00	3A4
MOTA	2409		VAL	349	43.834	14.402	-7.958	1.00	0.00	3A4
ATOM	2410	С	VAL	349	44.175	17.435	~7.201	1.00	0.00	3A4
ATOM	2411	0	VAL	349	44.934	16.990	-6.341	1.00	0.00	3A4 3A4
ATOM	2412	N CA	LEU	350 350	43.387 43.440	18.518 19.369	-6.988 -5.824	1.00	0.00	3A4
ATOM ATOM	2413 2414	CB	LEU	350	44.479	20.520	-6.024	1.00	0.00	3A4
ATOM	2415	CG	LEU	350	44.847	21.374	-4.785	1.00	0.00	3A4
ATOM	2416		LEU	350	45.497	20.539	-3.662	1.00	0.00	3A4
ATOM	2417		LEU	350	45.743	22.560	-5.187	1.00	0.00	3A4
MOTA	2418	С	LEU	350	42.042	19.913	-5.672	1.00	0.00	3A4
ATOM	2419	0	LEU	350	41.270	19.945	-6.631	1.00	0.00	3A4
ATOM	2420	N	GLN	351	41.689	20.372	-4.436	1.00	0.00	3A4
ATOM	2421	CA	GLN	351	40.404	20.942	-4.059	1.00	0.00	3A4
ATOM	2422	CB	GLN	351	40.005	20.645	-2.573	1.00	0.00	3A4 3A4
ATOM	2423	CG	GLN	351	40.814 42.269	21.289 20.816	-1.417 -1.386	1.00	0.00 0.00	3A4
ATOM ATOM	2424 2425	CD	GLN GLN	351 351	43.177	21.634	-1.520	1.00	0.00	3A4
ATOM	2426		GLN	351	42.505	19.487	-1.200	1.00	0.00	3A4
ATOM	2427	c	GLN	351	40.390	22.432	-4.305	1.00	0.00	3A4
ATOM	2428	o	GLN	351	41.399	23.112	-4.117	1.00	0.00	3A4
ATOM	2429	N	MET	352	39.214	22.962	-4.740	1.00	0.00	3A4
MOTA	2430	CA	MET	352	38.994	24.368	-5.014	1.00	0.00	3A4
MOTA	2431	СВ	MET	352	38.436	24.632	-6.438	1.00	0.00	3A4
MOTA	2432	CG	MET	352	38.472	26.097	-6.900	1.00	0.00	3A4
ATOM	2433	SD	MET	352	37.969	26.316	-8.633	1.00	0.00	3A4
ATOM	2434	CE	MET	352	38.075	28.129 24.911	-8.608	1.00	0.00 0.00	3A4 3A4
ATOM	2435 2436	C O	MET MET	352 352	38.113 38.636	25.287	-3.914 -2.866	1.00	0.00	3A4
ATOM ATOM	2437	N	GLU	353	36.765	25.000	-4.117	1.00	0.00	3A4
ATOM	2438	CA	GLU	353	35.914	25.749	-3.211	1.00	0.00	3A4
ATOM	2439	СВ	GLU	353	35.689	27.217	-3.688	1.00	0.00	3A4
MOTA	2440	CG	GLU	353	36.922	28.142	-3.627	1.00	0.00	3A4
MOTA	2441	ÇD	GLU	353	36.543	29.540	-4.126	1.00	0.00	3A4
MOTA	2442		GLU	353	36.622	30.504	-3.318	1.00	0.00	3A4
ATOM	2443	OE2		353	36.171	29.660	-5.325	1.00	0.00	3A4
ATOM	2444	C	GLU	353	34.592	25.102	-2.984	1.00	0.00	3A4 3A4
ATOM	2445 2446	O N	GLU TYR	353 354	34.078 33.979	25.104 24.537	-1.864 -4.047	1.00	0.00	3A4
ATOM ATOM	2447	CA	TYR	354	32.629	24.016	-3.996	1.00	0.00	3A4
ATOM	2448	СВ	TYR	354	31.928	24.005	-5.369	1.00	0.00	3A4
ATOM	2449	CG	TYR	354	31.880	25.395	-5.954	1.00	0.00	3A4
MOTA	2450	CD1	TYR	354	32.962	25.916	-6.691	1.00	0.00	3A4
ATOM	2451	CD2	TYR	354	30.740	26.199	-5.783	1.00	0.00	3A4
ATOM	2452		TYR	354	32.917	27.212	-7.224	1.00	0.00	3A4
ATOM	2453		TYR	354	30.683	27.496	-6.314	1.00	0.00	3A4
ATOM	2454		TYR	354	31.774	28.004	-7.035	1.00	0.00	3A4 3A4
ATOM ATOM	2455 2456	OH C	TYR TYR	354 354	31.722 32.592	29.310 22.628	-7.571 -3.428	1.00	0.00	384
ATOM	2457	Ö	TYR		31.575		-2.892	1.00	0.00	3A4
ATOM	2458	N	LEU	355	33.710	21.867	-3.466	1.00	0.00	3A4
ATOM	2459	CA	LEU	355	33.715	20.493	-2.996	1.00	0.00	3A4
MOTA	2460	СВ	LEU	355	34.970	19.771	-3.512	1.00	0.00	3A4
MOTA	2461	CG	LEU	355	34.521	18.784	-4.631	1.00	0.00	3A4
ATOM	2462		LEU	355	35.547	18.525	-5.749	1.00	0.00	3A4
ATOM	2463		LEU	355	33.945	17.479	-4.064	1.00	0.00	3A4
ATOM	2464	C	LEU	355	33.573	20.380	-1.485 -0.980	1.00	0.00	3A4 3A4
MOTA MOTA	2465 2466	0	LEU ASP	355 356	32.806 34.225	19.570 21.283	-0.721	1.00	0.00	3A4
ATOM	2467	N CA	ASP		34.070	21.466	0.714	1.00		3A4
ATOM	2468	CB	ASP	356	34.921	22.723	1.144	1.00		3A4
ATOM	2469	CG	ASP	356	35.819	22.461	2.358			3A4
ATOM	2470		ASP		35.262	22.182	3.454	1.00		3A4
ATOM	2471		ASP		37.067	22.560	2.214	1.00		3A4
ATOM	2472	С	ASP		32.651	21.700	1.182			3A4
ATOM	2473	0	ASP		32.180	21.110	2.149			3A4
ATOM	2474	N	MET	357	31.928	22.551	0.423			3A4
ATOM	2475	CA	MET		30.540	22.879	0.616			3A4
ATOM	2476	CB CG	MET MET		30.168 29.601	24.100 25.250	-0.239 0.627			3A4 3A4
MOTA	2477	CG	rae I	,,,	25.001	23.230	0.021	1.00	5.00	JA1

ATOM	2478	SD	MET	357	30.612	26.763	0.665	1.00	0.00	3A4
MOTA	2479	CE	MET	357	29.381	27.754	1.562	1.00	0.00	3A4
ATOM	2480	С	MET	357	29.622	21.737	0.289	1.00	0.00	3A4
ATOM	2481	0	MET	357	28.618	21.519	0.952 -0.714	1.00	0.00	3A4 3A4
ATOM	2482	N	VAL	358 358	29.995 29.302	20.909 19.693	-1.096	1.00	0.00	3A4
ATOM ATOM	2483 2484	CA CB	VAL VAL	358 358	29.848	19.071	-2.374	1.00	0.00	3A4
ATOM	2485		VAL	358	29.224	17.667	-2.681	1.00	0.00	3A4
ATOM	2486		VAL	358	29.530	20.074	-3.459	1.00	0.00	3A4
ATOM	2487	С	VAL	358	29.376	18.671	0.012	1.00	0.00	3A4
MOTA	2488	0	VAL	358	28.364	18.076	0.363	1.00	0.00	3A4
ATOM	2489	N	VAL	359	30.567	18.479	0.633	1.00	0.00	3A4
ATOM	2490	CA	VAL	359	30.783	17.579	1.758	1.00	0.00	3A4
ATOM	2491	CB	VAL	359	32.264	17.531	2.146 3.459	1.00	0.00	3A4 3A4
ATOM	2492		VAL VAL	359 359	32.553 33.043	16.768 16.854	1.004	1.00	0.00	3A4
ATOM ATOM	2493 2494	C	VAL	359	29.954	17.977	2.962	1.00	0.00	3A4
ATOM	2495	ŏ	VAL	359	29.303	17.151	3.591	1.00	0.00	3A4
ATOM	2496	N	ASN	360	29.903	19.287	3.263	1.00	0.00	3A4
ATOM	2497	CA	ASN	360	29.117	19.830	4.350	1.00	0.00	3A4
MOTA	2498	CB	ASN	360	29.412	21.328	4.537	1.00	0.00	3A4
MOTA	2499	CG	ASN	360	30.795	21.548	5.189	1.00	0.00	3A4
ATOM	2500		ASN	360	31.725	20.750	5.080	1.00	0.00	3A4
MOTA	2501		ASN	360	30.946	22.706	5.890	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2502 2503	C	ASN	360	27.624 26.891	19.645 19.274	4.147 5.060	1.00	0.00	3A4
ATOM	2504	N N	ASN GLU	360 361	27.149	19.820	2.890	1.00	0.00	3A4
ATOM	2505	CA	GLU	361	25.768	19.606	2.527	1.00	0.00	3A4
ATOM	2506	СВ	GLU	361	25.458	20.211	1.139	1.00	0.00	3A4
MOTA	2507	CG	GLU	361	24.026	19.998	0.629	1.00	0.00	3A4
ATOM	2508	CD	GLU	361	22.935	20.638	1.489	1.00	0.00	3A4
MOTA	2509		GLU	361	23.253	21.306	2.504	1.00	0.00	3A4
ATOM	2510		GLU	361	21.740	20.442	1.143	1.00	0.00 0.00	3A4 3A4
MOTA	2511	C	GLU	361	25.372 24.258	18.147 17.809	2.553 2.941	1.00	0.00	3A4
ATOM ATOM	2512 2513	O N	GLU Thr	361 362	26.285	17.210	2.205	1.00	0.00	3A4
ATOM	2514	CA	THR	362	26.034	15.779	2.269	1.00	0.00	3A4
ATOM	2515	СВ	THR	362	27.109	14.973	1.573	1.00	0.00	3A4
ATOM	2516	OG1	THR	362	27.154	15.360	0.208	1.00	0.00	3A4
MOTA	2517	CG2	THR	362	26.766	13.462	1.673	1.00	0.00	3A4
MOTA	2518	C	THR	362	25.886	15.303	3.702	1.00	0.00	3A4
ATOM	2519	0	THR	362	24.990	14.527	4.020 4.611	1.00	0.00	3A4 3A4
MOTA MOTA	2520 2521	N CA	LEU	363 363	26.722 26.677	15.835 15.555	6.026	1.00	0.00	3A4
ATOM	2522	СВ	LEU	363	27.934	16.102	6.729	1.00	0.00	3A4
ATOM	2523	CG	LEU	363	29.216	15.310	6.428	1.00	0.00	3A4
ATOM	2524		LEU	363	30.434	16.188	6.740	1.00	0.00	3A4
MOTA	2525	CD2	LEU	363	29.238	13.981	7.211	1.00	0.00	3A4
ATOM	2526	С	LEU	363	25.448	16.157	6.698	1.00	0.00	3A4
ATOM	2527	0	LEU	363	24.956	15.614	7.681	1.00	0.00	3A4 3A4
ATOM	2528 2529	N CA	ARG ARG	364 364	24.890 23.659	17.274 17.879	6.163 6.633	1.00	0.00	3A4
MOTA MOTA	2530	CB	ARG	364	23.446	19.303	6.082		0.00	3A4
ATOM	2531	CG	ARG	364	22.238	20.031	6.676		0.00	3A4
ATOM	2532	CD	ARG	364	22.212	21.544	6.417		0.00	3A4
MOTA	2533	NE	ARG	364	21.256	22.182	7.393		0.00	3A4
MOTA	2534	CZ	ARG	364	21.624	22.741	8.595		0.00	3A4
ATOM	2535		ARG	364	20.663	23.251	9.418		0.00	3A4
ATOM	2536		ARG	364	22.925 22.463	22.809 17.060	8.992 6.233			3A4 3A4
MOTA MOTA	2537 2538	С 0	ARG ARG	364 364	21.622	16.711	7.049			3A4
ATOM	2539		LEU	365	22.393	16.685	4.940			3A4
ATOM	2540	CA	LEU	365	21.267	15.979				3A4
MOTA	2541	СВ	LEU	365	21.247	16.050				3A4
ATOM	2542		LEU	365	19.879	16.592	2.326	1.00		3A4
MOTA	2543		LEU	365	19.837	16.585				3A4
MOTA	2544		LEU	365	18.607	15.874	2.828	_		3A4
ATOM	2545		LEU	365 365	21.135					3A4 3A4
ATOM ATOM	2546 2547		LEU PHE	365 366	20.029 22.252					3A4 3A4
ATOM	2547 2548		PHE		22.232					3A4
ATOM	2549		PHE		22.642					3A4
			_							

ATOM	2550	CG	PHE	366	21.503	11.244	3.297	1.00	0.00	3A4
MOTA	2551	CD1	PHE	366		11.861	2.035	1.00	0.00	3A4
MOTA	2552	CD2	PHE	366	20.363	10.498	3.651	1.00	0.00	3A4
ATOM	2553	CE1		366	20.455	11.742	1.150	1.00	0.00	3A4
ATOM	2554	CE2		366	19.278	10.377	2.773	1.00	0.00	3A4 3A4
ATOM	2555 2556	CZ	PHE PHE	366 366	19.325 23.116	11.000 12.273	1.520 6.585	1.00	0.00	· 3A4
ATOM ATOM	2557	С О	PHE	366	24.165	11.637	6.497	1.00	0.00	3A4
ATOM	2558	N	PRO	367	22.732	12.795	7.772	1.00	0.00	3A4
ATOM	2559	CA	PRO	367	23.466	12.674	9.011	1.00	0.00	3A4
ATOM	2560	CD	PRO	367	21.498	13.517	7.993	1.00	0.00	3A4
MOTA	2561	CB	PRO	367	22.894	13.739	9.935	1.00	0.00	3A4
ATOM	2562	CG	PRO	367	21.461	13.878	9.463 9.536	1.00	0.00	3A4 3A4
ATOM ATOM	2563 2564	с 0	PRO PRO	367 367	23.332 22.246	11.269 10.779	9.824	1.00	0.00	3A4
ATOM	2565	И	ILE	368	24.476	10.773	9.569	1.00	0.00	3A4
ATOM	2566	CA	ILE	368	24.602	9.143	9.718	1.00	0.00	3A4
ATOM	2567	СВ	ILE	368	25.992	8.818	9.131	1.00	0.00	3A4
MOTA	2568	CG2	ILE	368	27.160	9.306	10.024	1.00	0.00	3A4
ATOM	2569		ILE	368	26.230	7.413	8.553	1.00	0.00	3A4
ATOM	2570	CD	ILE	368	26.421	6.268	9.546	1.00 1.00	0.00	3A4 3A4
ATOM ATOM	2571 2572	C O	ILE	368 368	24.406 24.024	8.654 7.515	11.153 11.392	1.00	0.00	3A4
ATOM	2573	N	ALA	369	24.661	9.530	12.146	1.00	0.00	3A4
ATOM	2574	CA	ALA	369	24.719	9.183	13.542	1.00	0.00	3A4
ATOM	2575	СВ	ALA	369	26.067	9.640	14.141	1.00	0.00	3A4
MOTA	2576	С	ALA	369	23.654	9.859	14.360	1.00	0.00	3A4
ATOM	2577	0	ALA	369	23.267	10.991	14.104	1.00	0.00	3A4
ATOM ATOM	2578 2579	N CA	MET MET	370 370	23.265 22.422	9.221 9.803	15.511 16.560	1.00 1.00	0.00	3A4 3A4
ATOM	2580	CB	MET	370	20.964	9.264	16.470	1.00	0.00	3A4
ATOM	2581	CG	MET	370	19.910	10.113	17.209	1.00	0.00	3A4
ATOM	2582	SD	MET	370	18.173	9.663	16.885	1.00	0.00	3A4
ATOM	2583	CE	MET	370	18.081	10.195	15.146	1.00	0.00	3A4
ATOM	2584	C	MET	370	23.062	9.512	17.921	1.00	0.00	3A4
ATOM	2585 2586	O N	MET ARG	370 371	23.884 22.711	8.603 10.299	18.029 18.992	1.00	0.00	3A4 3A4
MOTA MOTA	2587	CA	ARG	371	23.356	10.277	20.307	1.00	0.00	3A4
ATOM	2588	СВ	ARG	371	24.430	11.405	20.437	1.00	0.00	3A4
MOTA	2589	CG	ARG	371	23.944	12.828	20.099	1.00	0.00	3A4
ATOM	2590	CD	ARG	371	25.049	13.888	20.216	1.00	0.00	3A4
ATOM	2591	NE	ARG	371	24.503	15.208	19.738	1.00	0.00	3A4 3A4
MOTA MOTA	2592 2593	CZ NH1	ARG	371 371	25.012 24.468	16.428 17.561	20.108 19.575	1.00	0.00	3A4
ATOM	2594		ARG	371	26.049	16.546	20.988	1.00	0.00	3A4
ATOM	2595	С	ARG	371	22.333	10.392	21.438	1.00	0.00	3A4
ATOM	2596	0	ARG	371	21.181	10.760	21.216	1.00	0.00	3A4
ATOM	2597	N	LEU	372	22.776	10.045	22.692	1.00	0.00	3A4
MOTA MOTA	2598 2599	CA CB	LEU	372 _. 372	22.016 21.964	9.951 8.482	23.936 24.512	1.00	0.00	3A4 3A4
ATOM	2600	CG	LEU	372	21.345	7.343	23.661	1.00	0.00	3A4
ATOM	2601		LEU	372	19.908	7.641		1.00	0.00	3A4
ATOM	2602		LEU	372	22.216	6.816	22.501	1.00	0.00	3A4
ATOM	2603	С	LEU	372	22.693	10.771	25.005	1.00	0.00	3A4
ATOM	2604	0	LEU	372	23.899 21.900	11.003 11.155	24.975 26.021	1.00	0.00	3A4 3A4
ATOM ATOM	2605 2606	N CA	GLU GLU	373 373	22.322	11.155	27.237	1.00	0.00	3A4
ATOM	2607	CB	GLU	373	22.131	13.344	27.172	1.00	0.00	3A4
ATOM	2608	CG	GLU	373	23.197	14.057	26.329	1.00	0.00	3A4
ATOM	2609	ÇĐ	GLU	373	23.009	15.577	26.343	1.00	0.00	3A4
ATOM	2610		GLU	373	23.722	16.250	25.553	1.00	0.00	3A4
ATOM	2611		GLU	373	22.167 21.466	16.090 11.241	27.128 28.351	1.00	0.00	3A4 3A4
MOTA MOTA	2612 2613	С 0	GLU	373 373	20.387	10.695	28.121		0.00	3A4
ATOM	2614	N	ARG	374	21.930	11.386	29.612		0.00	3A4
ATOM	2615	CA	ARG	374	21.138	11.043	30.774		0.00	3A4
ATOM	2616	СВ	ARG	374	21.532	9.678	31.420		0.00	3A4
ATOM	2617	CG	ARG	374	22.371	9.595	32.715		0.00	3A4
ATOM	2618 2619	CD NE	ARG		21.558 22.476	9.546 9.916	34.018 35.152			3A4 3A4
ATOM ATOM	2620	CZ	ARG ARG		22.476	9.595	36.465			3A4
ATOM	2621		ARG		23.147	10.010	37.405			3A4

ATOM	2622	NH2	ARG	374	21.156	8.879	36.860	1.00	0.00	3A4
ATOM	2623	С	ARG	374	21.272	12.200	31.721		0.00	3A4
MOTA	2624	0	ARG	374	22.360	12.720	31.947		0.00	3A4
MOTA	2625	N	VAL	375	20.152	12.629	32.340	1.00	0.00	3A4
MOTA	2626	CA	VAL	375	20.085	13.742	33.272	1.00	0.00	3A4
ATOM	2627	СВ	VAL	375	18.651	14.239	33.344	1.00	0.00	3A4
ATOM	2628	CG1		375	18.283	15.175	34.420	1.00	0.00 0.00	3A4 3A4
ATOM	2629	CG2		375	18.394 20.606	14.888	31.964 34.625	1.00	0.00	3A4
ATOM	2630 2631	С О	VAL VAL	375 375	20.173	12.325	35.197	1.00	0.00	3A4
ATOM ATOM	2632	И	CYS	376	21.593	14.058	35.166	1.00	0.00	3A4
ATOM	2633	CA	CYS	376	22.269	13.722	36.404	1.00	0.00	3A4
ATOM	2634	СВ	CYS	376	23.708	14.284	36.408	1.00	0.00	3A4
ATOM	2635	SG	CYS	376	24.721	13.423	35.165	1.00	0.00	3A4
ATOM	2636	С	CYS	376	21.525	14.230	37.618	1.00	0.00	3A4
MOTA	2637	0	CYS	376	21.699	13.713	38.720	1.00	0.00	3A4
MOTA	2638	N	LYS	377	20.691	15.268	37.426	1.00	0.00	3A4
MOTA	2639	CA	LYS	377	19.982	15.944	38.480	1.00	0.00	3A4
ATOM	2640	CB	LYS	377	20.773	17.167	38.996	1.00	0.00	3A4
ATOM	2641	CG	LYS	377	22.008	16.876	39.867	1.00	0.00	3A4
ATOM	2642	CD	LYS	377	21.695	16.179	41.198	1.00	0.00	3A4 3A4
ATOM	2643	CE	LYS	377	22.947	15.957	42.056	1.00	0.00 0.00	3A4
ATOM	2644	NZ	LYS	377	22.604 18.735	15.293	43.336 37.827	1.00 1.00	0.00	3A4
ATOM	2645	С	LYS	377	18.735	16.448 16.603	36.617	1.00	0.00	3A4
ATOM	2646	0	LYS LYS	377 378	17.690	16.839	38.593	1.00	0.00	3A4
ATOM	2647 2648	N CA	LYS	378	16.465	17.414	38.063	1.00	0.00	3A4
ATOM ATOM	2649	СВ	LYS	378	15.419	17.607	39.177	1.00	0.00	3A4
ATOM	2650	CG	LYS	378	15.088	16.287	39.895	1.00	0.00	3A4
ATOM	2651	CD	LYS	378	14.017	16.418	40.984	1.00	0.00	3A4
ATOM	2652	CE	LYS	378	13.613	15.082	41.625	1.00	0.00	3A4
ATOM	2653	NZ	LYS	378	14.747	14.462	42.352	1.00	0.00	3A4
ATOM	2654	С	LYS	378	16.741	18.741	37.382	1.00	0.00	3A4
ATOM	2655	0	LYS	378	17.545	19.524	37.877	1.00	0.00	3A4
ATOM	2656	N	ASP	379	16.172	18.960	36.183	1.00	0.00	3A4
ATOM	2657	CA	ASP	379	16.483	20.125	35.394	1.00	0.00	3A4
ATOM	2658	СВ	ASP	379	17.706	19.925	34.443	1.00	0.00	3A4
MOTA	2659	CG	ASP	379	17.527	19.059	33.183	1.00	0.00	3A4
ATOM	2660		ASP	379	17.455	17.817	33.330	1.00	0.00	3A4
ATOM	2661		ASP	379	17.475	19.634	32.063	1.00	0.00	3A4 3A4
ATOM	2662	С	ASP	379	15.250	20.543	34.652 34.415	1.00	0.00 0.00	3A4
ATOM	2663	0	ASP	379	14.333 15.216	19.776 21.819	34.247	1.00	0.00	3A4
ATOM	2664 2665	N CA	VAL VAL	380 380	14.098	22.398	33.548	1.00	0.00	3A4
MOTA MOTA	2666	CB	VAL	380	13.450	23.491	34.376	1.00	0.00	3A4
ATOM	2667		VAL	380	12.212	24.040	33.665	1.00	0.00	3A4
ATOM	2668		VAL	380	13.057	22.943	35.763	1.00	0.00	3A4
ATOM	2669	c	VAL	380	14.659	22.869	32.227	1.00	0.00	3A4
ATOM	2670	ō	VAL	380	15.521	23.743	32.201	1.00	0.00	3A4.
ATOM	2671	N	GLU	381	14.219	22.259	31.107	1.00	0.00	3A4
ATOM	2672	CA	GLU	381	14.653	22.560	29.760	1.00	0.00	3A4
MOTA	2673	СВ	GLU	381	15.044	21.298	28.989	1.00	0.00	3A4
MOTA	2674	CG	GLU	381	15.995	21.611	27.810	1.00	0.00	3A4
MOTA	2675	CD	GLU	381	16.331	20.375	26.965	1.00	0.00	3A4
ATOM	2676		GLU	381	17.063	20.564	25.958	1.00	0.00	3A4
ATOM	2677		GLU	381	15.873	19.246	27.284	1.00	0.00	3A4 3A4
ATOM	2678	С	GLU	381	13.495	23.231	29.052	1.00	0.00	3A4
MOTA	2679	0	GLU	381	12.355 13.715	22.802 24.405	29.042 28.468	1.00	0.00	3A4
ATOM	2680	N	ILE	382 382	12.690	25.313	27.960	1.00	0.00	3A4
MOTA MOTA	2681 2682	CA CB	ILE		11.956	24.945	26.638	1.00	0.00	3A4
ATOM	2683		ILE		10.525	25.549				3A4
ATOM	2684		llLE		12.874	25.434	25.467			3A4
ATOM	2685	CD.	ILE		12.229	25.497				3A4
ATOM	2686	c	ILE		11.919	25.809				3A4
ATOM	2687	ŏ	ILE		12.497	26.469				3A4
ATOM	2688	N	ASN	383	10.722	25.435				3A4
ATOM	2689	CA	ASN		10.349	25.838				3A4
ATOM	2690	ÇВ	ASN		9.806	27.330				3A4
MOTA	2691	CG	ASN		9.693	27.860				3A4
MOTA	2692		1 ASN		8.596	28.169				3A4
ATOM	2693	ND:	2 ASN	383	10.843	27.967	33.129	1.00	0.00	3A4

ATOM	2694	С	ASN	383	9.349	24.945	31.284	1.00	0.00	3A4
ATOM	2695	0	ASN	383	8.160	25.107	30.993		0.00	3A4
MOTA	2696	N	GLY	384	9.485	23.892	32.102	1.00	0.00	3A4
MOTA	2697	CA	GLY	384	8.315	22.984	32.156	1.00	0.00	3A4 3A4
ATOM ATOM	2698 2699	С 0	GLY GLY	384 384	8.276 7.285	22.292 21.764	30.798 30.297	1.00	0.00	3A4
ATOM	2700	N	MET	385	9.600	22.252	30.331	1.00	0.00	3A4
ATOM	2701	CA	MET	385	9.904	20.858	30.491	1.00	0.00	3A4
ATOM	2702	СВ	MET	385	10.648	20.273	29.245	1.00	0.00	3A4
ATOM	2703	CG	MET	385	10.078	18.932	28.749	1.00	0.00	3A4
ATOM	2704	SD	MET	385	10.271	17.522	29.885	1.00	0.00	3A4
MOTA	2705	CE	MET	385 385	8.674 10.673	16.747 20.574	29.504 31.772	1.00	0.00	3A4 3A4
ATOM ATOM	2706 2707	С 0	MET MET	385	11.823	20.374	31.867	1.00	0.00	3A4
ATOM	2708	N	PHE	386	10.077	19.903	32.767	1.00	0.00	3A4
ATOM	2709	CA	PHE	386	10.786	19.416	33.933	1.00	0.00	3A4
ATOM	2710	CB	PHE	386	9.854	19.471	35.160	1.00	0.00	3A4
ATOM	2711	CG	PHE	386	10.561	19.327	36.492	1.00	0.00	3A4
ATOM	2712		PHE PHE	386 386	10.905 10.861	20.467 18.057	37.242 37.026	1.00 1.00	0.00	3A4 3A4
MOTA MOTA	2713 2714		PHE	386	11.556	20.349	38.477	1.00	0.00	3A4
ATOM	2715		PHE	386	11.512	17.931	38.260	1.00	0.00	3A4
ATOM	2716	CZ	PHE	386	11.859	19.080	38.985	1.00	0.00	3A4
ATOM	2717	С	PHE	386	11.245	17.997	33.650	1.00	0.00	3A4
MOTA	2718	0	PHE	386	10.434	17.097	33.442	1.00	0.00	3A4
ATOM	2719	N	ILE	387	12.579	17.797	33.622 33.348	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	2720 2721	CA CB	ILE	387 387	13.234 14.381	16.542 16.682	32.335	1.00	0.00	3A4
MOTA	2722		ILE	387	14.760	15.256	31.874	1.00	0.00	3A4
ATOM	2723		ILE	387	13.940	17.566	31.142	1.00	0.00	3A4
MOTA	2724	CD	ILE	387	14.996	17.732	30.052	1.00	0.00	3A4
ATOM	2725	C	ILE	387	13.712	16.037	34.699	1.00	0.00	3A4
ATOM	2726 2727	O N	ILE PRO	387 388	14.542 13.230	16.701 14.898	35.311 35.231	1.00	0.00	3A4 3A4
ATOM ATOM	2728	CA	PRO	388	13.741	14.297	36.449	1.00	0.00	3A4
ATOM	2729	CD	PRO	388	11.827	14.522	35.038	1.00	0.00	3A4
ATOM	2730	СВ	PRO	388	12.685	13.264	36.864	1.00	0.00	3A4
ATOM	2731	CG	PRO	388	11.381	13.833	36.327	1.00	0.00	3A4
MOTA	2732	С	PRO	388	15.090	13.656	36.297	1.00	0.00	3A4 3A4
ATOM ATOM	2733 2734	O N	PRO LYS	388 389	15.481 15.825	13.246 13.516	35.212 37.416	1.00	0.00 0.00	3A4
ATOM	2735	CA	LYS	389	17.102	12.839	37.479	1.00	0.00	3A4
ATOM	2736	СВ	LYS	389	17.661	12.891	38.918	1.00	0.00	3A4
MOTA	2737	CG	LYS	389	16.754	12.453	40.092	1.00	0.00	3A4
MOTA	2738	CD	LYS	389	16.878	10.984	40.532	1.00	0.00	3A4
MOTA MOTA	2739 2740	CE NZ	LYS LYS	389 389	16.079 14.624	10.653 10.849	41.802 41.589	1.00	0.00	3A4 3A4
ATOM	2741	C	LYS	389	16.984	11.412	37.009	1.00	0.00	3A4
ATOM	2742		LYS	389	15.997	10.745	37.301	1.00	0.00	. 3A4
ATOM	2743	N	GLY	390	17.932	10.973	36.172	1.00	0.00	3A4
ATOM	2744	CA	GLY	390	17.963	9.654	35.593	1.00	0.00	3A4
MOTA	2745 2746	C	GLY GLY	390	17.174 17.046	9.470 8.351	34.332 33.839	1.00	0.00 0.00	3A4 3A4
MOTA MOTA	2747	О И	TRP	390 391	16.619	10.571	33.769	1.00	0.00	3A4
ATOM	2748	CA	TRP	391	15.850	10.544	32.546	1.00	0.00	3A4
ATOM	2749	СВ	TRP	391	14.930	11.760	32.448	1.00	0.00	3A4
ATOM	2750	CG	TRP	391	13.571	11.608	33.100	1.00		3A4
ATOM	2751		TRP	391	13.050	10.792	34.187	1.00		3A4 3A4
ATOM ATOM	2752 2753		TRP	391 391	12.458 11.305	12.068 11.618	32.439 33.025	1.00		3A4
ATOM	2754		TRP	391	11.634	10.839		1.00		3A4
ATOM	2755		TRP	391	13.655	10.032	35.188			'3A4
ATOM	2756	CZZ	TRP	391	10.825	10.153	35.005	1.00		3A4
ATOM	2757		TRP		12.843	9.345				3A4
ATOM	2758		TRP	391	11.446	9.404	36.011 31.369			3A4 3A4
ATOM ATOM	2759 2760	С 0	TRP TRP	391 391	16.783 17.769	10.563 11.289				3A4
ATOM	2761	N	VAL		16.466	9.736			_	3A4
ATOM	2762	CA	VAL		17.263	9.564				3A4
ATOM	2763	СВ	VAL	392	17.270	8.105				3A4
MOTA	2764		VAL		17.957	7.898				3A4
MOTA	2765	CG2	VAL	392	17.984	7.270	29.787	1.00	0.00	3A4

MOTA	2766	С	VAL	392	16.723	10.497	28.110	1.00	0.00	3A4
MOTA	2767	0	VAL	392	15.519	10.598	27.908	1.00	0.00	3A4
MOTA	2768	N	VAL	393	17.636	11.234	27.453	1.00	0.00	3A4
MOTA	2769	CA	VAL	393	17.333	12.226	26.455	1.00	0.00	3A4
ATOM	2770	CB	VAL	393	17.828	13.610	26.868	1.00	0.00	3A4
ATOM ATOM	2771 2772	CG1 CG2		393 393	17.556 17.145	14.652 14.023	25.780 28.194	1.00	0.00	3A4 3A4
ATOM	2773	C	VAL	393	17.143	11.735	25.192	1.00	0.00	3A4
ATOM	2774	o	VAL	393	19.147	11.327	25.196	1.00	0.00	3A4
ATOM	2775	N	MET	394	17.251	11.776	24.072	1.00	0.00	3A4
ATOM	2776	CA	MET	394	17.726	11.439	22.757	1.00	0.00	3A4
MOTA	2777	CB	MET	394	16.799	10.393	22.065	1.00	0.00	3A4
ATOM	2778	CG	MET	394	16.558	9.106	22.860	1.00	0.00	3A4
ATOM	2779	SD	MET	394	15.673	7.800	21.946	1.00	0.00	3A4
ATOM ATOM	2780 2781	CE C	MET MET	394 394	16.910 17.772	7.426 12.724	20.666 21.991	1.00 1.00	0.00	3A4 3A4
ATOM	2782	Ö	MET	394	16.799	13.464	21.947	1.00	0.00	3A4
ATOM	2783	N	ILE	395	18.916	13.023	21.347	1.00	0.00	3A4
ATOM	2784	CA	ILE	395	19.139	14.208	20.554	1.00	0.00	3A4
ATOM	2785	СВ	ILE	395	20.476	14.837	20.956	1.00	0.00	3A4
ATOM	2786	CG2		395	21.095	15.840	19.965	1.00	0.00	3A4
ATOM	2787	CG1	ILE	395	20.413	15.442	22.374	1.00	0.00	3A4
ATOM	2788	CD	ILE	395	20.802	14.496	23.518	1.00	0.00	3A4
ATOM	2789	C	ILE	395	19.146	13.747 13.239	19.102 18.627	1.00	0.00	3A4 3A4
ATOM ATOM	2790 2791	о И	ILE PRO	395 396	20.160 18.048	13.239	18.342	1.00	0.00	3A4
ATOM	2792	CA	PRO	396	18.027	13.792	16.906	1.00	0.00	3A4
ATOM	2793	CD	PRO	396	16.755	13.448	18.870	1.00	0.00	3A4
MOTA	2794	CB	PRO	396	16.531	13.829	16.546	1.00	0.00	3A4
MOTA	2795	CG	PRO	396	15.857	13.097	17.687	1.00	0.00	3A4
MOTA	2796	C	PRO	396	18.776	14.889	16.173	1.00	0.00	3A4
ATOM	2797	0	PRO	396	18.239	15.950	15.861	1.00	0.00	3A4
ATOM ATOM	2798 2799	N CA	SER	397 397	20.048 20.904	14.601 15.470	15.825 15.055	1.00	0.00	3A4 3A4
ATOM	2800	CB	SER SER	397	22.360	14.989	15.079	1.00	0.00	3A4 3A4
ATOM	2801	OG	SER	397	22.500	13.601	14.800	1.00	0.00	3A4
ATOM	2802	C	SER	397	20.417	15.595	13.635	1.00	0.00	3A4
ATOM	2803	0	SER	39 7	20.522	16.640	13.023	1.00	0.00	3A4
MOTA	2804	N	TYR	398	19.766	14.539	13.106	1.00	0.00	3A4
MOTA	2805	CA	TYR	398	19.026	14.496	11.862	1.00	0.00	3A4
ATOM	2806	CB	TYR	398	18.323	13.079 12.353	11.799	1.00	0.00	3A4 3A4
ATOM ATOM	2807 2808	CG CD1	TYR TYR	398 398	18.447 19.004	11.056	10.483 10.456	1.00	0.00	3A4 3A4
MOTA	2809			398	18.041	12.935	9.266	1.00	0.00	3A4
MOTA	2810		TYR	398	19.153	10.357	9.251	1.00	0.00	3A4
MOTA	2811	CE2	TYR	398	18.216	12.249	8.058	1.00	0.00	3A4
MOTA	2812	CZ	TYR	398	18.763	10.958	8.048	1.00	0.00	3A4
ATOM	2813	OH	TYR	398	18.924	10.266	6.829	1.00	0.00	3A4
MOTA	2814	C	TYR	398	17.923	15.540 16.207	11.741	1.00	0.00	3A4 3A4
ATOM ATOM	2815 2816	O N	TYR ALA	398 399	17.730 17.184	15.730	10.728 12.853	1.00	0.00	3A4
ATOM	2817	CA	ALA	399	16.116	16.686	12.969	1.00	0.00	3A4
ATOM	2818	СВ	ALA	399	15.263	16.409	14.206	1.00	0.00	3A4
ATOM	2819	С	ALA	399	16.594	18.122	13.028	1.00	0.00	3A4
ATOM	2820	0	ALA	399	15.939	19.008	12.501	1.00	0.00	3A4
MOTA	2821	N	LEU	400	17.795	18.377	13.599	1.00	0.00	3A4
ATOM	2822	CA	LEU	400	18.426	19.687 19.647	13.645	1.00	0.00	3A4 3A4
ATOM ATOM	2823 2824	CB CG	LEU	400 400	19.762 19.694	19.664	14.448 15.956	1.00	0.00	3A4 3A4
ATOM	2825		LEU	400	20.663	20.773	16.433	1.00	0.00	3A4
ATOM	2826		LEU	400	18.244	19.759	16.433	1.00	0.00	3A4
MOTA	2827	С	LEU	400	18.832	20.202	12.285		0.00	3A4
ATOM	2828	0	LEU	400	18.639	21.368	11.954	1.00	0.00	3A4
ATOM	2829	N	HIS	401	19.402	19.298	11.465	1.00	0.00	3A4
ATOM	2830	CA	HIS	401	19.852	19.556	10.124	1.00	0.00	3A4
MOTA MOTA	2831 2832	CG	HIS HIS	401 401	22.332 21.917	16.943 18.117	10.714 10.143	1.00	0.00	3A4 3A4
ATOM	2833	CB	HIS	401	20.572	18.319	9.559		0.00	3A4
ATOM	2834		HIS	401	24.123	18.219	10.505		0.00	3A4
ATOM	2835		HIS	401	23.023	18.893	10.033		0.00	3A4
ATOM	2836		HIS	401	23.659	17.057	10.914	1.00	0.00	3A4
MOTA	2837	С	HIS	401	18.745	19.836	9.125	1.00	0.00	3A4

MOTA	2838	0	HIS	401	18.970	20.398	8.056	1.00	0.00	3A4
ATOM	2839	N	ARG	402	17.513	19.410	9.474	1.00	0.00	3A4
ATOM	2840	CA	ARG	402	16.350	19.558	8.644	1.00	0.00	3A4
MOTA	2841	CB	ARG	402	15.632	18.220	8.410	1.00	0.00	3A4
ATOM	2842	CG	ARG	402	16.476	17.220	7.607	1.00	0.00	3A4
ATOM	2843	CD	ARG	402	15.663	15.992	7.176	1.00	0.00	3A4
ATOM	2844	NE	ARG	402	16.519	15.105	6.308	1.00	0.00	3A4
ATOM	2845	CZ	ARG	402	16.028	14.373	5.254	1.00	0.00	3A4
MOTA	2846	NH1	ARG	402	16.860	13.518	4.593	1.00	0.00	3A4
ATOM	2847	NH2	ARG	402	14.725	14.465	4.853	1.00	0.00	3A4
MOTA	2848	С	ARG	402	15.378	20.553	9.211	1.00	0.00	3A4
MOTA	2849	0	ARG	402	14.224	20.625	8.790	1.00	0.00	3A4
ATOM	2850	N	ASP	403	15.839	21.391	10.171	1.00	0.00	3A4
MOTA	2851	CA	ASP	403	15.031	22.422	10.772	1.00	0.00	3A4
MOTA	2852	СВ	ASP	403	15.642	22.973	12.085	1.00	0.00	3A4 3A4
ATOM	2853	CG	ASP	403	14.530	23.734	12.847	1.00	0.00	3A4
MOTA	2854		ASP	403	14.116	24.806	12.394	1.00	0.00	3A4
ATOM	2855		ASP	403	13.981	23.160	13.823	1.00	0.00	3A4
MOTA	2856	C	ASP	403	14.822	23.549	9.771	1.00	0.00	3A4
MOTA	2857	0	ASP	403	15.805	24.148	9.348 9.387	1.00	0.00	3A4
MOTA	2858	N	PRO	404	13.575	23.872		1.00	0.00	3A4
ATOM	2859	CA	PRO	404	13.256	24.866	8.377	1.00	0.00	3A4
ATOM	2860	CD	PRO	404	12.350	23.288	9.945 8.133	1.00	0.00	3A4
ATOM	2861	CB	PRO	404	11.749	24.727	9.445	1.00	0.00	3A4
ATOM	2862	CG	PRO	404	11.195	24.161 26.287	8.784	1.00	0.00	3A4
ATOM	2863	C	PRO	404	13.582 13.786	27.122	7.915	1.00	0.00	3A4
MOTA	2864	0	PRO	404	13.702	26.594	10.092	1.00	0.00	3A4
ATOM	2865	N CA	LYS LYS	405 405	14.102	27.890	10.588	1.00	0.00	3A4
ATOM	2866 2867	CB	LYS	405	13.708	28.082	12.078	1.00	0.00	3A4
ATOM ATOM	2868	CG	LYS	405	12.230	27.779	12.361	1.00	0.00	3A4
ATOM	2869	CD	LYS	405	11.862	27.931	13.843	1.00	0.00	3A4
ATOM	2870	CE	LYS	405	10.437	27.465	14.181	1.00	0.00	3A4
ATOM	2871	NZ	LYS	405	9.420	28.274	13.467	1.00	0.00	3A4
ATOM	2872	c	LYS	405	15.589	28.111	10.451	1.00	0.00	3A4
ATOM	2873	ŏ	LYS	405	16.040	29.247	10.435	1.00	0.00	3A4
ATOM	2874	N	TYR	406	16.387	27.031	10.326	1.00	0.00	3A4
ATOM	2875	CA	TYR	406	17.828	27.082	10.196	1.00	0.00	3A4
ATOM	2876	СВ	TYR	406	18.501	25.978	11.073	1.00	0.00	3A4
ATOM	2877	CG	TYR	406	18.818	26.481	12.466	1.00	0.00	3A4
MOTA	2878	CD1	TYR	406	17.845	27.049	13.316	1.00	0.00	3A4
ATOM	2879	CD2	TYR	406	20.123	26.324	12.973	1.00	0.00	3A4
MOTA	2880	CE1	TYR	406	18.180	27.502	14.601	1.00	0.00	3A4
ATOM	2881	CE2	TYR	406	20.465	26.758	14.261	1.00	0.00	3A4
MOTA	2882	CZ	TYR	406	19.493	27.354	15.076	1.00	0.00	3A4
ATOM	2883	ОН	TYR	406	19.831	27.781	16.379	1.00	0.00	3A4
ATOM	2884	С	TYR	406	18.238	26.911	8.742	1.00	0.00	3A4
ATOM	2885	0	TYR	406	19.185	27.556	8.293	1.00	0.00	3A4 3A4
ATOM	2886	N	TRP	407.	17.542	26.030	7.986	1.00	0.00	3A4
MOTA	2887	CA	TRP	407	17.869	25.728	6.609	1.00	0.00 0.00	3A4
MOTA	2888	CB	TRP	407	18.602	24.364	6.460 5.666	1.00	0.00	3A4
ATOM	2889	CG	TRP	407	19.890 20.082	24.534 24.159	4.293	1.00	0.00	3A4
ATOM	2890		TRP	407 407	21.050	25.141	6.063	1.00	0.00	3A4
ATOM	2891		l TRP	407	21.981	25.110	5.052	1.00	0.00	3A4
ATOM	2892 2893		l TRP 2 TRP	407	21.405	24.521	3.948	1.00	0.00	3A4
ATOM ATOM	2894		3 TRP		19.231	23.566	3.365	1.00	0.00	3A4
ATOM	2895		2 TRP		21.902	24.280	2.673	1.00	0.00	3A4
ATOM	2896		3 TRP		19.728	23.326	2.076		0.00	3A4
ATOM	2897		2 TRP		21.046	23.678	1.741	1.00	0.00	3A4
ATOM	2898	C	TRP		16.592	25.684	5.809	1.00		3A4
ATOM	2899	ŏ	TRP		15.735	24.831	6.029			3A4
ATOM	2900	N	THR		16.454	26.581	4.791	1.00		3A4
ATOM	2901	CA			15.311	26.691	3.895			3A4
ATOM	2902	CB			15.211	28.071	3.263			3A4
ATOM	2903		1 THR		16.432	28.505	2.662			3A4
ATOM	2904		2 THR		14.818	29.070	4.376			3A4
ATOM	2905		THR		15.392		2.839			3A4
ATOM	2906		THR		16.472		2.376			3A4
ATOM	2907		GLU	_	14.235	24.987	2.499			3A4
ATOM	2908				14.103					3A4
MOTA	2909				14.330	24.118	0.167	1.00	0.00	3A4

ATOM	2910	CG	GLU	409	13.370	25.190	-0.379		0.00	3A4
MOTA	2911		GLU	409	13.625	25.385	-1.878		0.00	3A4 3A4
MOTA	2912		GLU	409	12.698	25.099	-2.683 -2.236	1.00	0.00	3A4
ATOM	2913 2914	OE2 C	GLU GLU	409 409	14.752 15.001	25.821 22.657	2.097	1.00	0.00	3A4
ATOM ATOM	2915		GLU	409	15.858	22.218	1.334	1.00	0.00	3A4
ATOM	2916		PRO	410	14.886	22.233	3.369	1.00	0.00	3A4
ATOM	2917	CA	PRO	410	15.857	21.388	4.073	1.00	0.00	3A4
ATOM	2918	CD	PRO	410	13.663	22.414	4.165 5.504	1.00	0.00	3A4 3A4
MOTA	2919	CB CG	PRO PRO	410 410	15.298 13.783	21.307 21.467	5.357	1.00	0.00	3A4
ATOM ATOM	2920 2921	C	PRO	410	16.013	20.007	3.463	1.00	0.00	3A4
ATOM	2922	ō	PRO	410	17.048	19.368	3.620	1.00	0.00	3A4
MOTA	2923	N	GLU	411	15.001	19.530	2.723	1.00	0.00	3A4 3A4
ATOM	2924	CA	GLU	411	15.007	18.249 17.671	2.086 2.041	1.00	0.00	3A4 3A4
ATOM	2925 2926	CB CG	GLU GLU	411 411	13.575 12.398	18.662	1.868	1.00	0.00	3A4
ATOM ATOM	2927	CD	GLU	411	12.395	19.342	0.498	1.00	0.00	3A4
ATOM	2928	OE1		411	12.459	20.600	0.464	1.00	0.00	3A4
MOTA	2929	OE2		411	12.316	18.616	-0.530	1.00	0.00	3A4 3A4
MOTA	2930	C	GLU	411	15.637	18.272 17.227	0.712 0.076	1.00	0.00 0.00	3A4
ATOM	2931 2932	О И	GLU LYS	411 412	15.745 16.093	19.439	0.214	1.00	0.00	3A4
ATOM ATOM	2933	CA	LY\$	412	16.747	19.560	-1.069	1.00	0.00	3A4
ATOM	2934	СВ	LYS	412	16.319	20.855	-1.798	1.00	0.00	3A4
ATOM	2935	CG	LYS	412	14.842	20.918	-2.228	1.00	0.00	3A4 3A4
ATOM	2936	CD	LYS	412	14.489	20.264 18.726	-3.577 -3.601	1.00	0.00 0.00	3A4 3A4
ATOM	2937 2938	CE NZ	LYS LYS	412 412	14.483 13.990	18.220	-4.904	1.00	0.00	3A4
ATOM ATOM	2939	C	LYS	412	18.246	19.556	-0.876	1.00	0.00	3A4
ATOM	2940	ō	LYS	412	18.788	20.180	0.031	1.00	0.00	3A4
MOTA	2941	N	PHE	413	18.970	18.849	-1.771	1.00	0.00 0.00	3A4 3A4
MOTA	2942	CA	PHE	413	20.413	18.790 17.450	-1.784 -2.401	1.00	0.00	3A4
MOTA MOTA	2943 2944	CB CG	PHE	413 413	20.897 22.398	17.294	-2.423	1.00	0.00	3A4
MOTA	2945		PHE	413	23.168	17.227	-1.254	1.00	0.00	3A4
ATOM	2946		PHE	413	23.046	17.095	-3.661	1.00	0.00	3A4
ATOM	2947		PHE	413	24.550	16.999	-1.315	1.00	0.00 0.00	3A4 3A4
ATOM	2948		PHE	413 413	24.421 25.177	16.834 16.794	-3.726 -2.550	1.00	0.00	3A4
ATOM ATOM	2949 2950	CZ C	PHE	413	20.891	19.968	-2.586	1.00	0.00	3A4
ATOM	2951	ŏ	PHE	413	20.724	20.009	-3.801	1.00	0.00	3A4
MOTA	2952	N	LEU	414	21.483	20.957	-1.901	1.00	0.00	3A4 3A4
ATOM	2953	CA	LEU	414	21.933 20.902	22.177 23.301	-2.522 -2.306	1.00	0.00	3A4
ATOM ATOM	2954 2955	CB CG	LEU	414 414	21.169	24.700	-2.902	1.00	0.00	3A4
ATOM	2956		LEU	414	21.261	24.685	-4.441	1.00	0.00	3A4
ATOM	2957		LEU	414	20.079	25.663	-2.388	1.00	0.00	3A4
ATOM	2958	C	LEU	414	23.275	22.553		1.00	0.00	3A4. 3A4
ATOM	2959	O N	LEU	414 415	23.343 24.394	23.031 22.396	-0.834 -2.681	1.00	0.00	3A4
ATOM ATOM	2960 2961	CA	PRO PRO	415	25.721	22.710				3A4
ATOM	2962		PRO	415	24.457		-4.069			3A4
ATOM	2963		PRO	415	26.676					3A4 3A4
ATOM	2964		PRO	415	25.882					3A4
ATOM ATOM	2965 2966		PRO PRO	415 415	25.978 26.655		_			3A4
MOTA	2967		GLU	416	25.547				0.00	3A4
ATOM	2968		GLU	416	25.810					3A4
MOTA	2969		GLU	416	27.244					3A4 3A4
MOTA	2970		GLU	416	28.338 29.636					3A4
ATOM ATOM	2971 2972		GLU GLU		29.584					3A4
• ATOM	2973		2 GLU		30.704			1.00	0.00	3A4
MOTA	2974	С	GLU	416	24.818	27.126				3A4
MOTA	2975		GLU		24.357					3A4 3A4
ATOM	2976		ARG		24.555 23.940					3A4 3A4
MOTA MOTA	2977 2978				22.623					3A4
ATOM	2979				21.420	28.657	7 -4.370	1.00		3A4
MOTA	2980				20.160					3A4 3A4
ATOM	2981	l NE	ARG	417	19.654	29.550) -5.895	5 1.00	0.00	JAT

MOTA	2982	CZ	ARG	417	18.836	30.485			0.00	3A4
MOTA	2983	NH1		417	18.453	31.575			0.00	3A4
ATOM	2984	NH2	-	417	18.396	30.357	-4.021		0.00 0.00	3A4 3A4
ATOM ATOM	2985 2986		ARG ARG	417 417	23.675 23.277	30.614 31.695	-3.534 -3.966		0.00	3A4
ATOM	2987	N	PHE	418	23.883	30.380	-2.207	1.00	0.00	3A4
ATOM	2988	CA	PHE	418	23.598	31.253	-1.087	1.00	0.00	3A4
MOTA	2989	СВ	PHE	418	22.842	30.493	0.064	1.00	0.00	3A4
ATOM	2990	CG	PHE	418	23.400	29.109	0.354	1.00	0.00	3A4
ATOM	2991	CD1		418	24.479	28.931	1.245	1.00	0.00	3A4 3A4
ATOM ATOM	2992 2993	CD2	PHE	418 418	22.845 25.002	27.967 27.653	1.496	1.00	0.00	3A4
ATOM	2994		PHE	418	23.361	26.688	-0.007	1.00	0.00	3A4
MOTA	2995	CZ	PHE	418	24.442	26.532	0.869	1.00	0.00	3A4
ATOM	2996	С	PHE	418	24.891	31.865	-0.589	1.00	0.00	3A4
ATOM	2997	0	PHE	418	25.978	31.337	-0.822	1.00	0.00	3A4 3A4
ATOM	2998	N	SER	419	24.764	33.010 33.749	0.130 0.742	1.00	0.00	3A4
ATOM ATOM	2999 3000	CA CB	SER SER	419 419	25.850 26.168	35.084	0.003	1.00	0.00	3A4
ATOM	3001	OG	SER	419	26.610	34.824	-1.323	1.00	0.00	3A4
ATOM	3002	С	SER	419	25.419	34.042	2.158	1.00	0.00	3A4
ATOM	3003	0	SER	419	24.254	33.869	2.516	1.00	0.00	3A4
MOTA	3004	N	LYS	420	26.380	34.507	2.995	1.00	0.00	3A4 3A4
ATOM	3005	CA	LYS	420	26.162	34.853	4.383 5.338	1.00 1.00	0.00	3A4 3A4
ATOM	3006 3007	CB CG	LYS LYS	420 420	26.449 26.041	33.660 33.882	6.806	1.00	0.00	3A4
ATOM ATOM	3008	CD	LYS	420	25.973	32.611	7.673	1.00	0.00	3A4
ATOM	3009	CE	LYS	420	27.316	31.947	8.025	1.00	0.00	3A4
MOTA	3010	NZ	LYS	420	27.897	31.201	6.884	1.00	0.00	3A4
MOTA	3011	C	LYS	420	27.070	36.024	4.656	1.00	0.00	3A4 3A4
ATOM	3012	0	LYS	420	28.205	36.070 37.018	4.182 5.432	1.00	0.00	3A4
MOTA MOTA	3013 3014	N CA	LYS LYS	421 421	26.554 27.150	38.319	5.697	1.00	0.00	3A4
ATOM	3015	СВ	LYS	421	26.041	39.410	5.739	1.00	0.00	3A4
ATOM	3016	ÇG	LYS	421	26.518	40.872	5.751	1.00	0.00	3A4
MOTA	3017	CD	LYS	421	25.360	41.868	5.629	1.00	0.00	3A4
MOTA	3018	CE	LYS	421	25.821	43.332	5.619 5.492	1.00	0.00 0.00	3A4 3A4
MOTA MOTA	3019 3020	NZ C	LYS LYS	421 421	24.664 27.940	44.251 38.313	6.992	1.00	0.00	3A4
ATOM	3021	ō	LYS	421	28.871	39.099	7.165	1.00	0.00	3A4
ATOM	3022	N	ASN	422	27.572	37.398	7.933	1.00	0.00	3A4
MOTA	3023	CA	ASN	422	28.154	37.237	9.255	1.00	0.00	3A4
ATOM	3024	CB	ASN	422	27.020	37.047	10.319	1.00	0.00	3A4 3A4
ATOM	3025 3026	CG	ASN ASN	422 422	27.499 27.456	37.210 36.260	11.776 12.556	1.00	0.00	3A4
MOTA MOTA	3020		ASN	422	27.964	38.434	12.149	1.00	0.00	3A4
ATOM	3028	c	ASN	422	29.107	36.052	9.222	1.00	0.00	3A4
MOTA	3029	0	ASN	422	29.035	35.203	8.335	1.00	0.00	3A4
ATOM	3030		LYS	423	30.033	35.989	10.220	1.00	0.00	. 3A4 3A4
MOTA	3031	CA CB	LYS	423	31.052 32.450	34.968 35.576	10.382	1.00	0.00	3A4
MOTA MOTA	3032 3033		LYS LYS	423 423	33.030	36.450		1.00	0.00	3A4
ATOM	3034	CD	LYS	423	33.266	35.769		1.00	0.00	3A4
MOTA	3035		LYS	423	34.431	34.762		1.00	0.00	3A4
ATOM	3036		LYS	423	34.107	33.470	8.794	1.00		3A4
MOTA	3037		LYS	423	30.631	34.032	11.491 12.663	1.00	0.00	3A4 3A4
ATOM ATOM	3038 3039		LYS ASP	423 424	30.939 29.907	34.245 32.953		1.00		3A4
ATOM	3040		ASP	424	29.457	31.893				3A4
ATOM	3041		ASP	424	28.060	32.147		1.00	0.00	3A4
ATOM	3042		ASP	424	26.909			1.00		3A4
ATOM	3043		LASP	424	25.944	31.714				3A4 3A4
ATOM	3044		ASP	424	26.973 29.495		_			3A4 3A4
ATOM ATOM	3045 3046		ASP ASP	424 424	29.493					3A4
ATOM	3047		ASN		30.728					3A4
MOTA	3048		ASN		30.999	29.112	9.872	1.00		3A4
MOTA	3049		ASN		30.910					3A4
MOTA	3050		ASN		31.718					3A4 3A4
MOTA MOTA	3051 3052		l asn 2 asn		32.894 31.085					3A4
ATOM	3052		ASN ASN		32.363					3A4
		-								

3A4 3054 ASN 425 33.092 28.033 9.449 1.00 0.00 ATOM 0 11.570 1.00 0.00 3A4 32,734 28,773 ATOM 3055 N ILE 426 3A4 1.00 0.00 28.493 12,137 3056 CA ILE 426 34.043 ATOM 3A4 0.00 1.00 3057 CB ILE 426 34.648 29.716 12.854 ATOM ILE 426 36.105 29.402 13.297 1.00 0.00 3A4 3058 CG₂ ATOM 11.928 1.00 0.00 3A4 34.591 30.966 ATOM 3059 CG1 ILE 426 12.569 1.00 0.00 3A4 32,260 35.100 MOTA 3060 CD ILE 426 0.00 3A4 1.00 MOTA 3061 С ILE 426 33.870 27.289 13.047 0.00 3A4 34.107 26.155 12.633 1.00 3062 ILE 426 0 MOTA 14.315 1.00 0.00 3A4 427 33.447 27.532 3063 ASP ATOM N 0.00 3A4 33.204 26.537 15.348 1.00 ATOM 3064 CA ASP 427 1.00 0.00 3A4 3065 СВ ASP 427 34.320 26,450 16.444 ATOM 1.00 0.00 3A4 427 35.639 25.963 15.828 MOTA 3066 CG ASP 35.660 24.821 15.293 1.00 0.00 3A4 427 OD1 ASP ATOM 3067 1.00 0.00 3A4 36.643 26.722 15.888 OD2 ASP 427 MOTA 3068 15.973 1.00 0.00 3A4 31.841 26.813 ATOM 3069 C ASP 427 25.842 16.103 1.00 0.00 3A4 427 31.098 ATOM 3070 0 ASP 3A4 31.390 28.043 16.369 1.00 0.00 3071 N PRO 428 ATOM 16.637 1.00 0.00 3A4 PRO 428 29.983 28.361 ATOM 3072 CA 3A4 32.272 29.141 16.778 1.00 0.00 MOTA 3073 CD PRO 428 0.00 3A4 29.613 17.539 1.00 3074 СВ PRO 428 30.041 **ATOM** 0.00 3A4 31.359 30.308 17.172 1.00 **ATOM** 3075 CG PRO 428 3A4 PRO 428 29.245 28.611 15.321 1.00 0.00 3076 C ATOM 29.471 29.640 14.687 1.00 0.00 3A4 428 ATOM 3077 0 PRO 14.899 1.00 0.00 3A4 28.385 27.650 3078 TYR 429 ATOM N 3A4 0.00 27.755 1.00 ATOM 3079 CA TYR 429 27.649 13.596 3A4 3080 429 28.727 27.191 12.437 1.00 0.00 CB TYR ATOM 12.428 1.00 0.00 3A4 29.325 25.786 ATOM 3081 CG TYR 429 3A4 25.334 11.208 1.00 0.00 29.871 MOTA 3082 CD1 TYR 429 0.00 3A4 29.371 24.901 1.00 MOTA 3083 CD2 TYR 429 13.532 3A4 0.00 30.418 24.050 11.078 1.00 ATOM 3084 CE1 TYR 429 3A4 29.917 23.615 13.410 1.00 0.00 3085 CE₂ TYR 429 ATOM 0.00 3A4 30.437 23.186 12.181 1.00 429 ATOM 3086 CZ TYR 3A4 12.055 1.00 0.00 ATOM 3087 OH TYR 429 30.972 21.885 0.00 3A4 26.500 26.805 13.683 1.00 3088 TYR 429 MOTA С 0.00 3A4 429 25.984 26.542 14.769 1.00 MOTA 3089 0 TYR 26.004 26.339 12.499 1.00 0.00 3A4 3090 430 ATOM N ILE 24.912 25.392 12.301 1.00 0.00 3A4 CA 430 ATOM 3091 TLE 23.953 3A4 25.845 11.196 1.00 0.00 ATOM 3092 CB ILE 430 1.00 0.00 3A4 11.680 3093 CG2 430 23.323 27.171 ATOM ILE 3A4 0.00 430 24.623 26.004 9.800 1.00 ATOM 3094 CG1 ILE 3A4 26.472 8.700 1.00 0.00 3095 430 23.667 ATOM CD ILE 25.562 24.051 12.005 1.00 0.00 3A4 430 ATOM 3096 С ILE 12.016 1.00 0.00 3A4 26.789 23.977 ATOM 3097 0 ILE 430 **3A4** 22.951 1.00 0.00 3098 TYR 431 24.773 11.760 ATOM N 3A4 0.00 3099 CA TYR 431 25.198 21.604 11.414 1.00 ATOM 26.437 21.470 10.410 1.00 0.00 3A4 3100 431 ATOM CB TYR 26.384 0.00 3A4 22.218 9.097 1.00 ATOM 3101 CG TYR 431 3A4 25,.749 7.983 1.00 0,00 21.647 MOTA 3102 CD1 TYR 431 3A4 8.894 0.00 431 27.142 23.393 1.00 ATOM 3103 CD2 TYR 25.834 22.246 6.714 1.00 0.00 3A4 3104 CE1 TYR 431 ATOM 7.638 1.00 0.00 3A4 27.212 24.010 431 ATOM 3105 CE2 TYR 3A4 26.551 23.437 6.544 1.00 0.00 ATOM 3106 CZ TYR 431 0.00 3A4 26.632 24.036 5.267 1.00 **ATOM** 3107 OH TYR 431 3A4 12.688 1.00 0.00 25.647 20.889 ATOM 3108 С TYR 431 3A4 26.635 21.285 13.303 1.00 0.00 ATOM 3109 0 TYR 431 13.089 1.00 0.00 3A4 24.989 19.782 ATOM 3110 N THR 432 25.445 3A4 18.960 14.203 1.00 0.00 ATOM 3111 CA THR 432 15.316 1.00 0.00 3A4 24.381 18,938 MOTA 3112 THR 432 CB 3A4 14.826 1.00 0.00 432 23.070 18.659 ATOM 3113 OG1 THR 3A4 24.399 20.310 16.028 1.00 0.00 ATOM 3114 CG2 THR 432 13.781 25.810 17.558 1.00 0.00 3A4 3115 THR 432 ATOM c 16.648 14.576 1.00 0.00 3A4 25.565 ATOM 3116 0 THR 432 12,610 1.00 0.00 3A4 26.389 17.234 ATOM 3117 N PRO 433 3A4 12.240 1.00 0.00 ATOM 3118 CA PRO 433 26.601 15.849 3A4 PRO 433 27.173 18.101 11.724 1.00 0.00 ATOM 3119 CD 10.740 1.00 0.00 3A4 26.947 15.918 ATOM 3120 CB PRO 433 3A4 10.601 1.00 0.00 27.743 17.221 MOTA 3121 CG PRO 433 1.00 0.00 3A4 13,022 MOTA 3122 С PRO 433 27,748 15.209 3A4 0.00 27.771 13.993 13.150 1.00 ATOM 3123 0 PRO 433 3A4 28.673 16.013 13.587 1.00 0.00 3124 N PHE 434 ATOM 1.00 0.00 3A4

29.782

ATOM

3125

CA

PHE

434

15.548

14.382

ATOM	3126	СВ	PHE	434		16.257			0.00	3A4
MOTA	3127		PHE	434	31.591	15.810			0.00	3A4 3A4
MOTA	3128	CD1		434	31.353	16.451	11.514	1.00	0.00 0.00	3A4
MOTA	3129	CD2		434 434	32.354 31.813	14.754 16.203	12.363 10.200	1.00	0.00	3A4
ATOM	3130 3131	CE1		434	32.860	14.287	11.129	1.00	0.00	3A4
ATOM ATOM	3132	CZ	PHE	434	32.592	15.066	10.009	1.00	0.00	3A4
ATOM	3133	C	PHE	434	29.528	15.802	15.833	1.00	0.00	3A4
ATOM	3134	ō	PHE	434		15.663	16.655	1.00	0.00	3A4
ATOM	3135	N	GLY	435	28.291	16.210	16.191	1.00	0.00	3A4
ATOM	3136	CA	GLY	435	27.923	16.495	17.561	1.00	0.00	3A4
ATOM	3137	С	GLY	435	28.209	17.917	17.875	1.00	0.00	3A4
MOTA	3138	0	GLY	435	28.305	18.719	16.943	1.00	0.00	3A4
MOTA	3139	N	SER	436	28.348	18.248	19.183	1.00	0.00	3A4 3A4
ATOM	3140	CA	SER	436	28.384	19.623	19.578	1.00	0.00 0.00	3A4
ATOM	3141	CB	SER	436	26.947 26.948	20.258	19.543 19.489	1.00	0.00	3A4
ATOM ATOM	3142 3143	og C	SER SER	436 436	29.197	19.916	20.769	1.00	0.00	3A4
MOTA	3144	Ö	SER	436	30.134	20.642	20.647	1.00	0.00	3A4
ATOM	3145	N	GLY	437	28.951	19.486	21.973	1.00	0.00	3A4
ATOM	3146	CA	GLY	437	29.675	19.961	23.144	1.00	0.00	3A4
MOTA	3147	С	GLY	437	31.130	19.558	23.314	1.00	0.00	3A4
MOTA	3148	0	GLY	437	31.959	19.487	22.402	1.00	0.00	3A4
MOTA	3149	N	PRO	438	31.502	19.228	24.529	1.00	0.00	3A4
MOTA	3150	CA	PRO	438	32.875	18.727	24.776	1.00	0.00	3A4 3A4
ATOM	3151	CD	PRO	438	30.927	19.742	25.770	1.00	0.00 0.00	3A4
MOTA	3152	CB	PRO PRO	438 438	33.100 31.706	18.880 19.063	26.266 26.880	1.00	0.00	3A4
MOTA MOTA	3153 3154	CG C	PRO	438	33.099	17.295	24.317	1.00	0.00	3A4
ATOM	3155	Ö	PRO	438	34.230	16.824	24.348	1.00	0.00	3A4
ATOM	3156	N	ARG	439	32.033	16.608	23.850	1.00	0.00	3A4
MOTA	3157	CA	ARG	439	32.068	15.264	23.366	1.00	0.00	3A4
ATOM	3158	CB	ARG	439	30.905	14.467	23.961	1.00	0.00	3A4
MOTA	3159	CG	ARG	439	30.793	14.766	25.461	1.00	0.00	3A4
MOTA	3160	CD	ARG	439	30.197	13.690	26.366	1.00	0.00	3A4 3A4
ATOM	3161	NE	ARG	439	30.391	14.136	27.786 28.866	1.00	0.00	3A4
ATOM	3162	CZ	ARG ARG	439 439	30.091 30.342	13.354 13.836	30.116	1.00	0.00	3A4
MOTA MOTA	3163 3164		ARG	439	29.553	12.109	28.713	1.00	0.00	3A4
ATOM	3165	C	ARG	439	31.980	15.221	21.890	1.00	0.00	3A4
ATOM	3166	ō	ARG	439	31.776	14.165	21.309	1.00	0.00	3A4
ATOM	3167	N	ASN	440	32.201	16.364	21.200	1.00	0.00	3A4
ATOM	3168	CA	ASN	440	32.204	16.474	19.756	1.00	0.00	3A4
MOTA	3169	CB	ASN	440	32.625	17.886	19.354	1.00	0.00	3A4 3A4
MOTA	3170	CG	ASN	440	32.279	18.329	17.901 16.907	1.00	0.00	3A4
ATOM	3171		ASN	440 440	32.746 31.452	17.778 19.401	17.765	1.00	0.00	3A4
ATOM ATOM	3172 3173	C	ASN	440	33.216	15.539	19.171	1.00	0.00	3A4
ATOM	3174	ŏ	ASN	440	34.241	15.285	19.807	1.00	0.00	3A4
ATOM	3175	N	CYS	441	32.950	14.993	17.974	1.00	0.00	3A4
ATOM	3176	CA	CYS	441	33.782	14.009	17.328	1.00	0.00	3A4
ATOM	3177	CB	CYS	441	33.288	13.772	15.899	1.00	0.00	3A4
MOTA	3178	SG	CYS	441	34.028	12.338	15.029			3A4 3A4
MOTA	3179	C	CYS	441	35.241	14.414	17.264	1.00		3A4
ATOM	3180	0	CY\$	441	35.564 -36.131	15.528 13.531	16.866 17.746			3A4
ATOM ATOM	3181 3182	N CA	ILE	442 442	37.556	13.799				3A4
ATOM	3183	СВ	ILE	442	38.223	12.944				3A4
ATOM	3184		: ILE	442	38.388	11.476				3A4
ATOM	3185		ILE	442	39.528	13.570	19.391	1.00	0.00	3A4
ATOM	3186		ILE	442	39.336	14.819				3A4
MOTA	3187	С	ILE	442	38.181	13.605				3A4
ATOM	3188		ILE	442	39.180	14.220				3A4
ATOM	3189		GLY	443	37.524	12.758				3A4 3A4
MOTA	3190		GLY	443	37.942 37.399	12.408 13.252				3A4
ATOM	3191 3192		GLY GLY	443 443	37.399	12.902				3A4
ATOM ATOM	3192		MET	444	36.732	14.396				3A4
ATOM	3194		MET	444	36.082	15.266				3A4
ATOM	3195		MET	444	35.408			1.00	0.00	3A4
ATOM	3196		MET	444	36.294					3A4
MOTA	3197	SD	MET	444	35.375	18.583	15.04	1.00	0.00	3A4

ATOM	3198	CE	MET	444	36.695	18.911	16.244	1.00	0.00	3A4
ATOM	3199	С	MET	444	36.968	15.807	11.395	1.00	0.00	3A4
ATOM	3200	0	MET	444	36.570	15.844	10.236	1.00	0.00	3A4
MOTA	3201	N	ARG	445	38.230	16.170	11.727	1.00	0.00	3A4
ATOM	3202	CA	ARG	445	39.211	16.708	10.801	1.00	0.00	3A4
ATOM	3203	СВ	ARG	445	40.435	17.321	11.549	1.00	0.00	3A4
ATOM	3204	CG	ARG	445	40.058	18.332	12.647	1.00	0.00	3A4
ATOM	3205	CD	ARG	445	39.223	19.529	12.155	1.00	0.00	3A4 3A4
ATOM	3206	NE	ARG	445	38.880 37.901	20.389 21.351	13.341 13.313	1.00	0.00	3A4
MOTA MOTA	3207 3208	CZ NH1	ARG	445 445	37.643	22.071	14.443	1.00	0.00	3A4
ATOM	3209	NH2		445	37.171	21.600	12.186	1.00	0.00	3A4
ATOM	3210	C	ARG	445	39.695	15.651	9.828	1.00	0.00	3A4
ATOM	3211	ō	ARG	445	39.790	15.886	8.628	1.00	0.00	3A4
ATOM	3212	N	PHE	446	39.920	14.418	10.335	1.00	0.00	3A4
ATOM	3213	CA	PHE	446	40.293	13.256	9.549	1.00	0.00	3A4
MOTA	3214	СВ	PHE	446	40.683	12.116	10.501	1.00	0.00	3A4
MOTA	3215	CG	PHE	446	41.549	11.008	9.982	1.00	0.00	3A4
ATOM	3216	CD1		446	42.800	11.292	9.403	1.00	0.00	3A4
MOTA	3217	CD2		446	41.248	9.684		1.00	0.00	3A4
MOTA	3218	CE1		446	43.749	10.278	9.241	1.00	0.00	3A4 3A4
MOTA	3219		PHE	446	42.210	8.678	9.689	1.00 1.00	0.00	3A4
ATOM	3220 3221	CZ C	PHE	446 446	43.469 39.172	8.983 12.804	8.647	1.00	0.00	3A4
ATOM ATOM	3222	Ö	PHE	446	39.384	12.508	7.480	1.00	0.00	3A4
ATOM	3223	N	ALA	447	37.921	12.812	9.148	1.00	0.00	3A4
ATOM	3224	CA	ALA	447	36.738	12.472	8.393	1.00	0.00	3A4
ATOM	3225	СВ	ALA	447	35.499	12.464	9.272	1.00	0.00	3A4
ATOM	3226	С	ALA	447	36.489	13.392	7.228	1.00	0.00	3A4
ATOM	3227	0	ALA	447	36.216	12.950	6.120	1.00	0.00	3A4
MOTA	3228	N	LEU	448	36.656	14.715	7.427	1.00	0.00	3A4
MOTA	3229	CA	LEU	448	36.469	15.704	6.386	1.00	0.00	3A4
ATOM	3230	СВ	LEU	448	36.399	17.124	6.962	1.00	0.00	3A4
ATOM	3231	CG	LEU	448	35.089	17.408	7.731	1.00	0.00	3A4 3A4
MOTA	3232 3233		LEU	448	35.223 33.842	18.721 17.445	8.515 6.826	1.00	0.00	3A4
ATOM ATOM	3233	CDZ	LEU	448 448	37.561	15.661	5.351	1.00	0.00	3A4
ATOM	3235	ŏ	LEU	448	37.299	15.865	4.175	1.00	0.00	3A4
ATOM	3236	N	MET	449	38.806	15.319	5.746	1.00	0.00	3A4
ATOM	3237	CA	MET	449	39.935	15.178	4.853	1.00	0.00	3A4
MOTA	3238	CB	MET	449	41.269	15.033	5.617	1.00	0.00	3A4
MOTA	3239	CG	MET	449	41.841	16.358	6.130	1.00	0.00	3A4
MOTA	3240	SD	MET	449	43.382	16.135	7.075	1.00	0.00	3A4
MOTA	3241	CE	MET	449	43.701	17.904	7.332	1.00	0.00	3A4
ATOM	3242	c	MET	449	39.772	13.984	3.951	1.00	0.00	3A4 3A4
ATOM	3243 3244	O N	MET	449	39.956 39.332	14.095 12.829	2.746 4.502	1.00	0.00	3A4
ATOM ATOM	3244	CA	ASN ASN	450 450	39.098	11.625	3.740	1.00	0.00	3A4
ATOM	3246	CB	ASN	450	38.915	10.385	4.623	1.00	0.00	3A4.
ATOM	3247	CG	ASN	450	37.685	10.130	5.531	1.00	0.00	3A4
ATOM	3248		ASN	450	36.512	10.268	5.191	1.00	0.00	3A4
ATOM	3249	ND2	ASN	450	37.990	9.606	6.751	1.00	0.00	3A4
MOTA	3250	С	ASN	450	37.976	11.740	2.750	1.00	0.00	3A4
ATOM	3251	0	ASN	450	38.095	11.281	1.623		0.00	3A4
MOTA	3252	N	MET	451	36.874	12.422	3.129		0.00	3A4
ATOM	3253	CA	MET	451	35.744	12.687	2.267	1.00	0.00	3A4
ATOM	3254	CB	MET	451	34.596	13.445	3.021	1.00	0.00	3A4 3A4
ATOM ATOM	3255 3256	CG SD	MET MET	451 451	33.788 32.502	12.610 13.565	4.010 4.863		0.00	3A4
ATOM	3257	CE	MET	451	33.061	13.383	6.570		0.00	3A4
MOTA	3258	C	MET	451	36.081	13.580	1.106		0.00	3A4
ATOM	3259	ō	MET	451	35.746	13.314	-0.041		0.00	3A4
ATOM	3260	N	LYS		36.821	14.667	1.389		0.00	3A4
MOTA	3261	CA	LYS		37.237	15.652	0.424			3A4
ATOM	3262	СВ	LYS		37.854	16.860	1.154		0.00	3A4
MOTA	3263	CG	LYS		37.750	18.227	0.470		0.00	3A4
MOTA	3264	CD	LYS		38.346	19.380			0.00	3A4
ATOM	3265	CE	LYS		38.006	19.391	2.808			3A4
ATOM	3266	NZ	LYS		36.543	19.337				3A4 3A4
ATOM	3267	C	LYS		38.228	15.110 15.335				3A4
ATOM ATOM	3268 3269	O N	LYS LEU		38.108 39.207	14.309				3A4
A I OIS	3203	14	PEU	733	33.201	14.303	0.102	1.00	Ų. UU	5.11

ATOM	3270	CA	LEU	453	40.212	13.676	-0.927	1.00	0.00	3A4
ATOM	3271	СВ	LEU	453	41.342	13.071	-0.061	1.00	0.00	3A4
MOTA	3272	CG	LEU	453	42.298	14.219	0.403	1.00	0.00	3A4
ATOM	3273	CD1		453	43.187	13.854	1.595	1.00	0.00	3A4
ATOM	3274	CD2		453	43.191	14.764	-0.734 -1.845	1.00	0.00	3A4 3A4
ATOM ATOM	3275 3276	С 0	LEU	453 453	39.621 39.939	12.644 12.613	-3.026	1.00	0.00	3A4
ATOM	3277	N	λLA	454	38.662	11.829	-1.353	1.00	0.00	3A4
ATOM	3278	CA	ALA	454	37.935	10.847	-2.131	1.00	0.00	3A4
MOTA	3279	СВ	ALA	454	37.013	9.992	-1.240	1.00	0.00	3 n 4
ATOM	3280	С	ALA	454	37.093	11.464	-3.225	1.00	0.00	3A4
ATOM	3281	0	ALA	454	37.181	11.055	-4.371	1.00	0.00	3A4
ATOM ATOM	3282 3283	N CA	LEU	455	36.307 35.457	12.514 13.201	-2.904 -3.852	1.00	0.00	3A4 3A4
ATOM	3284	CB	LEU	455 455	34.480	14.157	-3.157	1.00	0.00	3A4
ATOM	3285	CG	LEU	455	33.366	13.559	-2.303	1.00	0.00	3A4
ATOM	3286	CD1		455	32.576	14.761	-1.760	1.00	0.00	3A4
ATOM	3287	CD2	LEU	455	32.474	12.556	-3.064	1.00	0.00	3A4
ATOM	3288	C	LEU	455	36.203	14.018	-4.886	1.00	0.00	3A4
MOTA	3289	0	LEU	455	35.736	14.147	-6.009	1.00	0.00	3A4 3A4
ATOM ATOM	3290 3291	N CA	ILE	456 456	37.412 38.284	14.540 15.264	-4.555 -5.474	1.00	0.00	3A4
ATOM	3292	CB	ILE	456	39.413	16.061	-4.749	1.00	0.00	3A4
ATOM	3293		ILE	456	40.832	16.074	-5.412	1.00	0.00	3A4
MOTA	3294		ILE	456	39.003	17.537	-4.565	1.00	0.00	3A4
MOTA	3295	CD	ILE	456	38.041	17.823	-3.423	1.00	0.00	3A4
ATOM	3296	C	ILE	456	38.894	14.318	-6.496	1.00	0.00	3A4
ATOM ATOM	3297 3298	O N	I LE ARG	456 457	39.099 39.181	14.677 13.066	-7.647 -6.083	1.00	0.00 0.00	3A4 3A4
ATOM	3299	CA	ARG	457	39.859	12.081	-6.895	1.00	0.00	3A4
ATOM	3300	СВ	ARG	457	40.758	11.186	-6.025	1.00	0.00	3A4
MOTA	3301	CG	ARG	457	41.905	12.005	-5.430	1.00	0.00	3A4
MOTA	3302	CD	ARG	457	42.735	11.300	-4.341	1.00	0.00	3A4
MOTA	3303	NE	ARG	457	43.559	12.343	-3.632	1.00	0.00	3A4
ATOM ATOM	3304 3305	CZ	ARG ARG	457 457	44.624 45.148	12.985 14.087	-4.211 -3.601	1.00 1.00	0.00 0.00	3A4 3A4
ATOM	3306		ARG	457	45.174	12.558	-5.385	1.00	0.00	3A4
ATOM	3307	С	ARG	457	38.924	11.235	-7.722	1.00	0.00	3A4
ATOM	3308	0	ARG	457	39.246	10.873	-8.848	1.00	0.00	3A4
MOTA	3309	N	VAL	458	37.713	10.918	-7.207	1.00	0.00	3A4
ATOM	3310	CA	VAL	458	36.711	10.092	-7.872	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	3311 3312	CB CG1	VAL VAL	458 458	35.631 34.290	9.662 9.133	-6.887 -7.471	1.00	0.00	3A4
ATOM	3313		VAL	458	36.253	8.556	-6.006	1.00	0.00	3A4
MOTA	3314	С	VAL	458	36.101	10.798	-9.063	1.00	0.00	3A4
MOTA	3315	0	VAL	458	36.040		-10.146	1.00	0.00	3A4
ATOM	3316	N	LEU	459	35.685	12.071	-8.900	1.00	0.00	3A4
ATOM ATOM	3317 3318	CA CB	LEU	459 459	34.979 34.354	12.841 14.096	-9.906 -9.255	1.00	0.00	3A4 3A4
ATOM	3319	CG	LEU	459	33.225	13.778	-8.265	1.00	0.00	3A4
ATOM	3320		LEU	459	32.786	15.037	-7.500	1.00	0.00	3A4
MOTA	3321	CD2	LEU	459	32.041	13.132	-8.991	1.00	0.00	3A4
ATOM	3322	C	LEU	459	35.826		-11.060	1.00	0.00	3A4
ATOM	3323	0	LEU	459	35.319		-12.136	1.00	0.00	3A4
ATOM ATOM	3324 3325	N CA	GLN GLN	460 460	37.158 38.070		-10.874 -11.927	1.00	0.00	3A4 3A4
ATOM	3326	СВ	GLN	460	39.373		-11.376	1.00	0.00	3A4
ATOM	3327	CG	GLN	460	39.106		-10.736	1.00	0.00	3A4
MOTA	3328	CD	GLN	460	40.408		-10.160	1.00	0.00	3A4
MOTA	3329		GLN	460	41.430		-10.237	1.00	0.00	3A4
ATOM	3330		GLN	460	40.380	17.515	-9.575	1.00	0.00	3A4
MOTA MOTA	3331 3332	C O	GLN GLN	460 460	38.365 38.683		-12.815 -13.990		0.00	3A4 3A4
ATOM	3333	N	ASN	461	38.258		-12.266		0.00	3A4
ATOM	3334	CA	ASN	461	38.598		-12.957	1.00	0.00	3A4
MOTA	3335	СВ	ASN		39.328		-12.018		0.00	3A4
ATOM	3336	CG	ASN	461	40.725		-11.730			3A4
ATOM	3337		ASN		41.364		-12.617			3A4 3A4
MOTA MOTA	3338 3339	C ND2	ASN ASN		41.239 37.402		-10.482 -13.562			3A4
ATOM	3340	ŏ	ASN		37.588		-14.451			3A4
ATOM	3341	N	PHE		36.167		-13.107			3A4

ATOM	3342	CA	PHE	462	34.983	8.975	-13.533	1.00	0.00	3A4
ATOM	3343	СВ	PHE	462	34.346		-12.354	1.00	0.00	3A4
ATOM	3344	CG	PHE	462	35.274	7.073	-11.873	1.00	0.00	3A4
ATOM	3345	CD1	PHE	462	35.686	6.051	-12.745	1.00	0.00	3A4
ATOM	3346	CD2		462	35.718		-10.540	1.00	0.00	3A4
MOTA	3347	CE1		462	36.530		-12.307	1.00	0.00	3A4
ATOM	3348	CE2		462	36.561		-10.089	1.00	0.00	3A4
ATOM	3349	CZ	PHE	462	36.972		-10.978	1.00	0.00	3A4
ATOM	3350	C	PHE	462 462	33.836		-14.135	1.00	0.00	3A4 3A4
ATOM ATOM	3351 3352	о И	PHE	463	33.734 32.784		-13.828 -15.007	1.00	0.00	3A4
ATOM	3353	CA	SER	463	31.446		-15.542	1.00	0.00	3A4
ATOM	3354	CB	SER	463	31.400		-17.094	1.00	0.00	3A4
ATOM	3355	OG	SER	463	32.293		-17.565	1.00	0.00	3A4
ATOM	3356	С	SER	463	30.513		~15.014	1.00	0.00	3A4
ATOM	3357	0	SER	463	30.243	7.578	-15.673	1.00	0.00	3A4
MOTA	3358	N	PHE	464	30.012	8.774	-13.767	1.00	0.00	3A4
MOTA	3359	CA	PHE	464	29.251		-13.078	1.00	0.00	3A4
ATOM	3360	СВ	PHE	464	29.689		-11.603	1.00	0.00	3A4
MOTA	3361	CG	PHE	464	29.600		-10.565	1.00	0.00	3A4
ATOM	3362	CD1		464	30.780	9.102	-9.999	1.00	0.00	3A4
ATOM	3363	CD2		464	28.364	8.952	-9.990	1.00	0.00	3A4 3A4
ATOM	3364	CE1	PHE	464 464	30.727 28.310	9.958 9.832	-8.891 -8.899	1.00	0.00	3A4
ATOM ATOM	3365 3366	CE2	PHE	464	29.493	10.333	-8.347	1.00	0.00	3A4
ATOM	3367	C	PHE	464	27.768		-13.199	1.00	0.00	3A4
ATOM	3368	ŏ	PHE	464	27.238		-13.175	1.00	0.00	3A4
ATOM	3369	N	LYS	465	27.076		-13.331	1.00	0.00	3A4
ATOM	3370	CA	LYS	465	25.646	6.719	-13.439	1.00	0.00	3A4
ATOM	3371	СВ	LYS	465	25.197	6.398	-14.891	1.00	0.00	3A4
ATOM	3372	CG	LYS	465	25.553		-15.915	1.00	0.00	3A4
MOTA	3373	CD	LYS	465	25.067		-17.333	1.00	0.00	3A4
ATOM	3374	CE	LYS	465	25.438		-18.374	1.00	0.00	3A4
ATOM	3375	NZ	LYS	465	26.910		-18.512	1.00	0.00	3A4 3A4
ATOM	3376	C O	LYS	465 465	25.212 25.982		-12.507 -12.254	1.00	0.00	3A4
ATOM ATOM	3377 3378	N	LYS PRO	466	23.983		-11.985	1.00	0.00	3A4
ATOM	3379	CA	PRO	466	23.422		-11.249	1.00	0.00	3A4
ATOM	3380	CD	PRO	466	23.090		-11.993	1.00	0.00	3A4
ATOM	3381	СВ	PRO	466	22.300		-10.405	1.00	0.00	3A4
ATOM	3382	CG	PRO	466	21.827	6.358	-11.228	1.00	0.00	3A4
MOTA	3383	С	PRO	466	22.906		-12.228	1.00	0.00	3A4
MOTA	3384	0	PRO	466	22.333		-13.264	1.00	0.00	3A4
ATOM	3385	N	CYS	467	23.088		-11.890	1.00	0.00	3A4
ATOM	3386	CA	CYS	467	22.624		-12.667	1.00	0.00	3A4 3A4
ATOM	3387	CB SG	CYS	467	23.617 23.434		-12.501 -13.674	1.00	0.00	3A4
ATOM ATOM	3388 3389	C	CYS CYS	467 467	21.212		-12.220	1.00	0.00	3A4
ATOM	3390	ŏ	CYS	467	20,555		-12.834	1.00	0.00	3A4
ATOM	3391	N	LYS	468	20.726		-11.130	1.00	0.00	3A4
ATOM	3392	CA	LYS	468	19.389		-10.573	1.00	0.00	3A4
ATOM	3393	СВ	LYS	468	19.406	1.410	-9.027	1.00	0.00	3A4
ATOM	3394	CG	LYS	468	20.290	0.367		1.00	0.00	3A4
MOTA	3395	CD	LYS	468	20.136	0.413		1.00	0.00	3A4
ATOM	3396	CE	LYS	468	21.077	-0.534		1.00	0.00	3A4
ATOM	3397	NZ	LYS	468	20.807	-0.485			0.00	3A4
ATOM	3398	C	LYS	468	18.586		9 -11.148 9 -11.548		0.00	3A4 3A4
ATOM	3399 3400	0	LYS	468 469	19.145 17.238		3 -11.348		0.00	3A4
ATOM ATOM	3401	N CA	GLU GLU	469	16.301		7 -11.832		0.00	3A4
ATOM	3402	CB	GLU	469	15.428		-12.905		0.00	3A4
ATOM	3403	CG	GLU	469	16.234		-14.000		0.00	3A4
ATOM	3404	CD	GLU	469	17.104		2 -14.780		0.00	3A4
ATOM	3405		GLU	469	16.530	3.642	2 -15.407	1.00	0.00	3A4
ATOM	3406	OE2		469	18.355		1 -14.761		0.00	3A4
ATOM	3407	С	GLU	469	15.433		2 -10.753		0.00	3A4
MOTA	3408	0	GLU	469	15.841	3.909				3A4
ATOM	3409	N	THR	470	14.183		2 -11.133			3A4
ATOM	3410	CA	THR		13.125		2 -10.289			3A4 3A4
ATOM	3411	CB	THR	470	12.400		7 -10.998 7 -10.138			3A4 3A4
ATOM ATOM	3412		THR THR		11.519 11.657		7 -10.138 7 -12.286			3A4
VI OW	3413	CG2		7,0	11.037	J.44	. 12.200		2.00	

ATOM	3414	С	THR	470	12.198	3.578	-9.882	1.00	0.00	3A4
ATOM	3415	0	THR	470	11.456	3.677	-8.906		0.00	3A4
MOTA	3416	N	GLN	471	12.279		-10.640		0.00	3A4
MOTA	3417	CA	GLN	471	11.670		-10.385	1.00	0.00	3A4
MOTA	3418	СВ	GLN	471	10.997		-11.656	1.00	0.00	3A4 3A4
ATOM	3419	CG	GLN	471	11.811		-12.967 -14.119	1.00	0.00	3A4 3A4
ATOM	3420 3421	CD	GLN GLN	471 471	10.976 10.763	-1.106		1.00	0.00	3A4
MOTA MOTA	3422		GLN	471	10.489		-15.035	1.00	0.00	3A4
ATOM	3423	C	GLN	471	12.773	0.276	-9.839	1.00	0.00	3A4
ATOM	3424	ŏ	GLN	471	13.605	-0.249		1.00	0.00	3A4
ATOM	3425	N	ILE	472	12.809	0.178	-8.475	1.00	0.00	3A4
ATOM	3426	CA	ILE	472	13.847	-0.369	-7.600	1.00	0.00	3A4
ATOM	3427	CB	ILE	472	14.451	-1.737	-7.993	1.00	0.00	3A4
ATOM	3428		ILE	472	15.447	-2.232	-6.907	1.00	0.00	3A4
MOTA	3429		ILE	472	13.359	-2.820	-8.240	1.00	0.00	3A4
ATOM	3430	CD	ILE	472	12.440	-3.129	-7.050	1.00	0.00	3A4 3A4
ATOM	3431	С	ILE	472	14.926	0.710	-7.400	1.00 1.00	0.00 0.00	3A4 3A4
ATOM	3432	0	ILE	472	15.870 14.837	0.760 1.594	-8.188 -6.373	1.00	0.00	3A4
ATOM	3433 3434	N CA	PRO PRO	473 473	15.865	2.553	-5.978	1.00	0.00	3A4
ATOM ATOM	3435	CD	PRO	473	13.607	1.778	-5.600	1.00	0.00	3A4
ATOM	3436	СВ	PRO	473	15.047	3.657	-5.263	1.00	0.00	3A4
ATOM	3437	CG	PRO	473	13.885	2.910	-4.607	1.00	0.00	3A4
ATOM	3438	c	PRO	473	16.926	1.936	-5.117	1.00	0.00	3A4
ATOM	3439	0	PRO	473	17.147	0.726	-5.098	1.00	0.00	3A4
ATOM	3440	N	LEU	474	17.606	2.821	-4.384	1.00	0.00	3A4
MOTA	3441	CA	LEU	474	18.692	2.518	-3.506	1.00	0.00	3A4
ATOM	3442	СВ	LEU	474	19.658	3.718	-3.467	1.00	0.00	3A4
ATOM	3443	CG	LEU	474	20.935	3.548	-2.623	1.00	0.00 0.00	3A4 3A4
ATOM	3444		LEU	474	22.187	3.637	-3.503 -1.472	1.00	0.00	3A4
ATOM	3445 3446	CD2	LEU	474 474	20.962 18.157	4.569 2.198	-2.136	1.00	0.00	3A4
ATOM ATOM	3447	Ö	LEU	474	17.397	2.966	-1.547	1.00	0.00	3A4
ATOM	3448	N	LYS	475	18.561	1.016	-1.612	1.00	0.00	3A4
ATOM	3449	CA	LYS	475	18.133	0.502	-0.330	1.00	0.00	3A4
ATOM	3450	СВ	LYS	475	18.199	-1.049	-0.249	1.00	0.00	3A4
ATOM	3451	CG	LYS	475	17.520	-1.656	0.999	1.00	0.00	3A4
ATOM	3452	CD	LYS	475	17.579	-3.189	1.074	1.00	0.00	3A4
MOTA	3453	CE	LYS	475	18.981	-3.776	1.311	1.00	0.00	3A4
MOTA	3454	NZ	LYS	475	19.572	-3.282	2.580	1.00	0.00	3A4
MOTA	3455	C	LYS	475	18.961	1.086	0.775	1.00	0.00 0.00	3A4 3A4
ATOM	3456	0	LYS	475	20.173 18.276	0.909 1.798	0.825 1.695	1.00	0.00	3A4
MOTA MOTA	3457 3458	N CA	LEU LEU	476 476	18.860	2.419	2.855	1.00	0.00	3A4
ATOM	3459		· LEU	476	18.422	3.903	3.070	1.00	0.00	3A4
ATOM	3460	CG	LEU	476	16.930	4.243	3.360	1.00	0.00	3A4
ATOM	3461		LEU	476	16.813	5.725	3.764	1.00	0.00	3A4
ATOM	3462	CD	LEU	476 .	15.956	3.930	2.201	1.00	0.00	3A4
ATOM	3463	С	LEU	476	18.580	1.579	4.038	1.00	0.00	3A4
MOTA	3464	0	LEU	476	17.524	0.970		1.00	0.00	3A4
MOTA	3465	N	SER	477	19.543	1.495		1.00	0.00	3A4 3A4
ATOM	3466	CA	SER	477	19.480 20.807	0.545		1.00	0.00 0.00	3A4
ATOM	3467 3468	CB OG	SER SER	477 477	20.584	-0.220 -1.554		1.00	0.00	3A4
ATOM ATOM	3469	C	SER	477	18.826	1.150		1.00	0.00	3A4
ATOM	3470	ŏ	SER	477	18.936	2.334		1.00	0.00	3A4
ATOM	3471	N	LEU	478	18.068	0.282		1.00	0.00	3A4
ATOM	3472	CA		478	17.386	0.588	9.132	1.00	0.00	3A4
ATOM	3473	СВ	LEU	478	16.072	-0.245			0.00	3A4
ATOM	3474	CG		478	15.314	-0.208				3A4
MOTA	3475		1 LEU	478	14.954	1.206				3A4
MOTA	3476		2 LEU	478	14.057	-1.098				3A4
ATOM	3477	C	LEU	478	18.338	0.280				3A4 3A4
ATOM	3478	0	LEU	478	18.566	-0.855 1.308				3A4
ATOM	3479 3480	N CA	GLY GLY	479 479	18.982 19.983	1.119				3A4
ATOM ATOM	3480	CA	GLY		19.558	1.665				3A4
ATOM	3482	0	GLY		19.405	0.936				3A4
ATOM	3483	N	GLY		19.416	2.996				3A4
ATOM	3484	CA			19.205	3.607	14.623	1.00	0.00	3A4
ATOM	3485		GLY		20.442	4.355		1.00	0.00	3A4

ATOM	3486	0	GLY	480	20.430	5.574	14.961	1.00	0.00	3A4
MOTA	3487	N	LEU	481	21.566	3.643	15.196	1.00	0.00	3A4
ATOM	3488	CA	LEU	481	22.833	4.218	15.597	1.00	0.00	3A4
ATOM	3489	CB	LEU	481	23.634	3.303	16.586	1.00	0.00	3A4
ATOM	3490	CG	LEU	481	23.971	1.830	16.194	1.00	0.00	3A4
ATOM	3491	CD1		481	25.057	1.273	17.135	1.00	0.00	3A4
ATOM	3492	CD2		481	22.767	0.861	16.168	1.00	0.00	3A4
ATOM	3493	Ċ.	LEU	481	23.664	4.637	14.398	1.00	0.00	3A4
ATOM	3494	0.	LEU	481	24.121 23.838	5.774 3.733	14.349 13.398	1.00	0.00	3A4 3A4
ATOM ATOM	3495 3496	N CA	LEU	482 482	24.486	3.733	12.124	1.00	0.00	3A4
MOTA	3497	СВ	LEU	482	25.613	2.951	11.765	1.00	0.00	3A4
ATOM	3498	CG	LEU	482	26.965	3.067	12.517	1.00	0.00	3A4
ATOM	3499	CD1		482	27.722	4.365	12.213	1.00	0.00	3A4
ATOM	3500	CD2		482	26.897	2.808	14.028	1.00	0.00	3A4
ATOM	3501	С	LEU	482	23.378	3.835	11.115	1.00	0.00	3A4
ATOM	3502	0	LEU	482	22.784	2.766	11.044	1.00	0.00	3A4
ATOM	3503	N	GLN	483	23.090	4.887	10.291	1.00	0.00	3A4
ATOM	3504	CA	GLN	483	22.131	4.849	9.194	1.00	0.00	3A4
MOTA	3505	СВ	GLN	483	21.199	6.105	9.194	1.00	0.00	3A4
ATOM	3506	CG	GLN	483	20.316	6.274	10.449	1.00	0.00	3A4
ATOM	3507	CD	GLN	483	19.134	5.295	10.458 9.605	1.00	0.00 0.00	3A4 3A4
ATOM ATOM	3508 3509	OE1 NE2		483 483	18.982 18.236	4.423 5.459	11.467	1.00	0.00	3A4
ATOM	3510	C	GLN	483	22.916	4.815	7.900	1.00	0.00	3A4
ATOM	3511	ŏ	GLN	483	23.541	5.820	7.606	1.00	0.00	3A4
ATOM	3512	N	PRO	484	22.951	3.748	7.093	1.00	0.00	3A4
ATOM	3513	CA	PRO	484	23.817	3.721	5.925	1.00	0.00	3A4
ATOM	3514	CD	PRO	484	22.874	2.409	7.687	1.00	0.00	3A4
ATOM	3515	CB	PRO	484	24.769	2.558	6.262	1.00	0.00	3A4
ATOM	3516	CG	PRO	484	23.861	1.520	6.915	1.00	0.00	3A4
MOTA	3517	С	PRO	484	23.035	3.412	4.673	1.00	0.00	3A4
ATOM	3518	0	PRO	484	21.816	3.307	4.680	1.00	0.00	3A4
ATOM	3519	N	GLU	485	23.773	3.212	3.562	1.00	0.00	3A4
ATOM	3520	CA	GLU	485	23.248	2.558	2.383	1.00	0.00	3A4 3A4
ATOM	3521 3522	CB	GLU	485	23.098 24.327	3.493 4.316	1.177 0.781	1.00	0.00	3A4
ATOM ATOM	3522	CG CD	GLU	485 485	24.829	3.771	-0.540	1.00	0.00	3A4
ATOM	3524		GLU	485	24.837	4.541	-1.536	1.00	0.00	3A4
ATOM	3525		GLU	485	25.209	2.571	-0.567	1.00	0.00	3A4
ATOM	3526	C	GLU	485	24.043	1.288	2.206	1.00	0.00	3A4
ATOM	3527	0	GLU	485	25.260	1.289	2.296	1.00	0.00	3A4
ATOM	3528	N	LYS	486	23.368	0.126	2.027	1.00	0.00	3A4
MOTA	3529	CA	LYS	486	24.038	-1.172	1.973	1.00	0.00	3A4
ATOM	3530	СВ	LYS	486	23.286	-2.272	2.791	1.00	0.00	3A4
ATOM	3531	CG	LYS	486	24.070	-3.558	3.141	1.00	0.00	3A4
ATOM	3532	CD	LYS	486	24.136	-4.672	2.074	1.00	0.00	3A4
ATOM ATOM	3533	CE	LYS	486	22.782	-5.249 -5.839	1.626	1.00	0.00	3A4 3A4
ATOM	3534 3535	NZ C	LYS LYS	486 486	22.037 24.427	-1.507	2.765 0.545	1.00	0.00	3A4.
ATOM	3536	ŏ	LYS	486	25.595	-1.841	0.334	1.00	0.00	3A4
ATOM	3537	N	PRO	487	23.564		-0.475	1.00	0.00	3A4
ATOM	3538	CA	PRO	487	23.980	-1.646	-1.846	1.00	0.00	3A4
ATOM	3539	CD	PRO	487	22.127	-1.666	-0.334	1.00	0.00	3A4
ATOM	3540	СВ	PRO	487	22.967	-2.687	-2.354	1.00	0.00	3A4
MOTA	3541	ÇG	PRO	487	21.658	-2.329	-1.638	1.00	0.00	3A4
ATOM	3542	С	PRO	487	23.927	-0.353	-2.647	1.00	0.00	3A4
MOTA	3543	0	PRO	487	22.999	0.443	-2.510	1.00	0.00	3A4
MOTA	3544	N	VAL	488	24.915	-0.147	-3.541	1.00	0.00	3A4
ATOM	3545	CA	VAL	488	24.946	1.001	-4.417	1.00	0.00	3A4
ATOM	3546	CB	VAL	488	25.614	2.234 1.920	-3.794 -3.030	1.00	0.00	3A4 3A4
ATOM ATOM	3547 3548		VAL VAL	488 488	26.927 25.731	3.431	-3.030 -4.776	1.00	0.00	3A4
ATOM	3549	C	VAL	488	25.663	0.556	-5.657	1.00	0.00	3A4
ATOM	3550	ò	VAL	488	26.886	0.485	-5.692	1.00	0.00	3A4
ATOM	3551	N	VAL	489	24.905	0.264	-6.743	1.00	0.00	3A4
ATOM	3552	CA	VAL	489	25.452	-0.202	-8.007	1.00		3A4
MOTA	3553	CB	VAL	489	24.587	-1.266	-8.687	1.00		3A4
MOTA	3554		VAL	489	25.369	-1.938	-9.848	1.00		3A4
MOTA	3555		VAL	489	24.212	-2.339	-7.638	1.00		3A4
ATOM	3556	C	VAL		25.702	0.999	-8.916	1.00		3A4
MOTA	3557	0	VAL	489	24.854	1.864	-9.093	1.00	0.00	3A4

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MOTA	3558	N	LEU	490	26.915	1.064 -9.4		0.00	3A4
ATOM	3559	CA	LEU	490	27.387	2.104 -10.3		0.00	3A4
ATOM	3560	CB	LEU	490	28.695	2.765 -9.8 3.732 -10.7		0.00 0.00	3A4 3A4
ATOM ATOM	3561 3562	CG CD1	LEU	490 490	29.556 30.364	4.675 -9.8		0.00	3A4
ATOM	3563	CD2		490	30.579	3.092 -11.6		0.00	3A4
ATOM	3564	C	LEU	490	27.689	1.443 -11.7		0.00	3A4
ATOM	3565	0	LEU	490	28.311	0.382 -11.7	14 1.00	0.00	3A4
MOTA	3566	N	LYS	491	27.223	2.080 -12.8		0.00	3A4
ATOM	3567	CA	LYS	491	27.177	1.589 -14.1		0.00	3A4
ATOM	3568 3569	CB CG	LYS LYS	491 491	25.982 25.687	2.230 -14.9 1.704 -16.3		0.00 0.00	3A4 3A4
ATOM ATOM	3570	CD	LYS	491	25.319	0.219 -16.4		0.00	3A4
ATOM	3571	CE	LYS	491	25.043	-0.263 -17.8		0.00	3A4
ATOM	3572	NZ	LYS	491	24.678	-1.699 -17.8	99 1.00	0.00	3A4
ATOM	3573	С	LYS	491	28.494	1.812 -14.9		0.00	3A4
ATOM	3574	0	LYS	491	29.380	0.964 -14.8		0.00	3A4
ATOM	3575	N	VAL	492	28.641	2.966 -15.6 3.255 -16.5		0.00 0.00	3A4 3A4
ATOM ATOM	3576 3577	CA CB	VAL VAL	492 492	29.700 29.112	3.889 -17.8		0.00	3A4
ATOM	3578		VAL	492	28.415	5.242 -17.5		0.00	3A4
ATOM	3579		VAL	492	30.130	3.946 -19.0		0.00	3A4
ATOM	3580	С	VAL	492	30.777	4.082 -15.8	398 1.00	0.00	3A4
MOTA	3581	0	VAL	492	30.519	4.769 -14.9		0.00	3A4
MOTA	3582	N	GLU	493	32.030	3.983 -16.4		0.00	3A4
ATOM	3583	CA	GLU	493	33.215 33.962	4.574 -15.8 3.566 -14.9		0.00 0.00	3A4 3A4
ATOM ATOM	3584 3585	CB CG	GLU	493 493	34.397	2.206 -15.5		0.00	3A4
ATOM	3586	CD	GLU	493	35.792	2.272 -16.1		0.00	3A4
ATOM	3587		GLU	493	36.769	2.568 -15.4	102 1.00	0.00	3A4
ATOM	3588	OE2	GLU	493	35.901	2.024 -17.3		0.00	3A4
MOTA	3589	С	GLU	493	34.100	5.031 -16.9		0.00	3A4
ATOM	3590	0	GLU	493	33.928	4.629 -18.1		0.00	3A4 3A4
MOTA MOTA	3591 3592	N CA	SER	494 494	35.109 36.209	5.874 -16.0 6.283 -17.0		0.00	3A4
ATOM	3593	CB	SER	494	36.076	7.748 -18.0		0.00	3A4
MOTA	3594	OG	SER	494	35.765	8.692 -16.9		0.00	3A4
ATOM	3595	С	SER	494	37.455	6.059 -16.	647 1.00	0.00	3A4
MOTA	3596	0	SER	494	37.360	5.784 -15.		0.00	3A4
MOTA	3597	N	ARG	495	38.664	6.138 -17.3		0.00	3A4
ATOM	3598 3599	CA CB	ARG	495 495	39.886 40.090	5.740 -16.5 4.192 -16.5		0.00	3A4 3A4
MOTA MOTA	3600	CG	ARG	495	39.845	3.452 -17.		0.00	3A4
ATOM	3601	CD	ARG	495	39.764	1.935 -17.		0.00	3A4
ATOM	3602	NE	ARG	495	39.301	1.272 -18.	966 1.00	0.00	3A4
MOTA	3603	CZ	ARG	495	38.710	0.032 -18.		0.00	3A4
ATOM	3604		ARG	495	38.289	-0.478 -20.		0.00	3A4
ATOM	3605 3606	NHZ C	ARG ARG	495 495	38.527 41.073	-0.702 -17. 6.436 -17.		0.00	3A4 3A4
ATOM ATOM	3607	. 0	ARG	495	41.144	6.643 -18.		0.00	3A4
ATOM	3608	N	ASP	496	42.044	6.804 -16.		0.00	3A4
ATOM	3609	CA	ASP	496	43.290	7.471 -16.		0.00	3A4
MOTA	3610	CB	ASP	496	43.159	9.025 -16.			3A4
ATOM	3611	CG	ASP	496	42.410	9.788 -15.			3A4
ATOM	3612		ASP	496	43.070	10.614 -15.			3A4 3A4
MOTA MOTA	3613 3614	C	ASP ASP	496 496	41.179 44.272	9.574 -15. 7.071 -15.			3A4
ATOM	3615	ŏ	ASP	496	44.432	5.882 -15.			3A4
ATOM	3616	N	GLY	497	44.958	8.050 -14.			3A4
MOTA	3617	CA	GLY	497	45.950	7.790 -13.			3A4
MOTA	3618	¢	GLY	497	46.123	9.024 -13.			3A4
MOTA	3619	0	GLY	497	46.262	10.127 -13.			3A4
MOTA MOTA	3620 3621	N CA	THR THR	498 498	46.127 46.355	8.846 -11. 9.879 -10.			3A4 3A4
ATOM	3622	CB	THR	498	45.075		995 1.00		3A4
ATOM	3623		THR	498	44.194		600 1.00		3A4
ATOM	3624		THR	498	44.332	11.355 -10.	957 1.00	0.00	3A4
ATOM	3625	С	THR		47.290		640 1.00		3A4
ATOM	3626	0	THR		47.189		326 1.00		3A4
ATOM	3627	N	VAL		48.205 49.121		074 1.00 014 1.00		3A4 3A4
ATOM ATOM	3628 3629	CA CB	VAL	499 499	50.272		476 1.00		3A4
A . Ota	5023		****	.,,	50.2.72	0.020 0.			

ATOM	3630	CG1	VAL	499	51.133	9.436	-9.607	1.00	0.00	3A4
ATOM	3631	CG2		499	51.110	8.313	-7.273	1.00	0.00	3A4
ATOM	3632	c	VAL	499	49.614	11.021	-7.391	1.00	0.00	3A4
ATOM	3633	ŏ	VAL	499	49.977	11.961	-8.097	1.00	0.00	3A4
	3634		SER	500	49.647	11.075	-6.030	1.00	0.00	3A4
ATOM		N					-5.269	1.00	0.00	3A4
ATOM	3635	CA	SER	500	50.251	12.152			0.00	3A4
MOTA	3636	СВ	SER	500	49.434	13.486	-5.230	1.00		
ATOM	3637	OG	SER	500	48.086	13.306	-4.816	1.00	0.00	3A4
ATOM	3638	С	SER	500	50.524	11.618	-3.882	1.00	0.00	3A4
ATOM	3639	0	SER	500	49.694	10.933	-3.286	1.00	0.00	3A4
ATOM	3640	N	GLY	501	51.736	11.945	-3.355	1.00	0.00	3A4
MOTA	3641	CA	GLY	501	52.249	11.543	-2.061	1.00	0.00	3A4
ATOM	3642	С	GLY	501	53.489	10.727	-2.291	1.00	0.00	3A4
ATOM	3643	0	GLY	501	54.576	11.087	-1.841	1.00	0.00	3A4
ATOM	3644	N	ALA	502	53.331	9.596	-3.020	1.00	0.00	3A4
ATOM	3645	CA	ALA	502	54.406	8.722	-3.424	1.00	0.00	3A4
ATOM	3646	СВ	ALA	502	54.772	7.642	-2.379	1.00	0.00	3A4
	3647		ALA	502	53.912	8.031	-4.704	1.00	0.00	3A4
MOTA		C				8.364	-5.800	1.00	0.00	3A4
MOTA	3648		ALA	502	54.439					3A4
MOTA	3649	OT2	ALA	502	52.987	7.178	-4.607	1.00	0.00	JAY
TER	3650		ALA	502						
HETATM		FE	HEM	600	33.118	10.391	15.288	1.00	0.00	HEM
HETATM	3652	NA	HEM	600	31.497	11.115	16.171	1.00	0.00	HEM
HETATM	3653	NB	HEM	600	32.274	10.658	13.514	1.00	0.00	HEM
HETATM	3654	NC	HEM	600	34.752	9.684	14.430	1.00	0.00	HEM
HETATM	3655	ND	HEM	600	33.949	10.106	17.065	1.00	0.00	HEM
HETATM		C1A	HEM	600	31.254	11.251	17.515	1.00	0.00	HEM
НЕТЛТМ			HEM	600	29.887	11.659	17.752	1.00	0.00	HEM
HETATM			HEM	600	29.316	11.871	16.542	1.00	0.00	HEM
НЕТАТМ			HEM	600	30.322	11.523	15.568	1.00	0.00	HEM
HETATM			HEM	600	31.012	11.136	13.233	1.00	0.00	HEM
HETATM			HEM	600	30.761	11.218	11.804	1.00	0.00	HEM
					31.901	10.761	11.185	1.00	0.00	HEM
HETATM			HEM	600					0.00	HEM
HETATM			HEM	600	32.828	10.426	12.273	1.00		
HETATM			HEM	600	35.044	9.645	13.089	1.00	0.00	HEM
HETATM			HEM	600	36.395	9.168	12.838	1.00	0.00	HEM
HETATM			HEM	600	36.920	8.833	14.067	1.00	0.00	HEM
HETATM	3667	C4C	HEM	600	35.879	9.167	15.033	1.00	0.00	HEM
HETATM	3668	C1D	HEM	600	35.150	9.494	17.358	1.00	0.00	HEM
HETATM	3669	C2D	HEM	600	35.382	9.408	18.787	1.00	0.00	HEM
HETATM	3670	C3D	HEM	600	34.329	10.035	19.375	1.00	0.00	HEM
HETATM	3671	C4D	HEM	600	33.438	10.439	18.306	1.00	0.00	HEM
HETATM	3672	CHA	HEM	600	32.186	10.978	18.500	1.00	0.00	HEM
HETATM			HEM	600	30.115	11.530	14.204	1.00	0.00	HEM
HETATM			HEM	600	34.131	9.963	12.102	1.00	0.00	HEM
HETATM			HEM	600	36.032	9.062	16.407	1.00	0.00	HEM
HETATM			HEM	600	27.911	12.344	16.281	1.00	0.00	HEM
HETATM			HEM	600	29.208	11.695	19.088	1.00	0.00	HEM
HETATM			HEM	600	29,154	13.045	19.638	1.00	0.00	HEM
-						13.237	20.946	1.00	0.00	HEM
HETATM			HEM	600	28.459			1.00	0.00	HEM
HETATM			HEM	600	28.097	12.278	21.566			HEM
HETATM			HEM	600	28.217	14.323	21.438	1.00	0.00	
HETATM			HEM	600	29.483	11.742	11.185	1.00	0.00	HEM
HETATM			HEM	600	32.219	10.602	9.818	1.00	0.00	HEM
HETATM		CBE	HEM	600	31.527	10.978	8.735		0.00	HEM
HETATM	3685	CMC	HEM	600	37.047	9.116	11.471	1.00	0.00	HEM
HETATM	3686	CAC	HEM	600	38.159	8.288	14.465	1.00	0.00	HEM
HETATM	3687	CBC	HEM:	600	39.265	8.069	13.758	1.00	0.00	HEM
HETATM			HEM	600	36.499	8.680	19.483	1.00	0.00	HEM
HETATM			HEM	600	34.101	10.253	20.849	1.00	0.00	HEM
HETATM			HEM	600	34.689	11.583	21.366		0.00	HEM
HETATM			HEM	600	34.355	11.863	22.843		0.00	HEM
HETATM			HEM	600	35.050	12.735	23.424			HEM
HETATM) HEM	600	33.381	11.284	23.380			HEM
END	. 5053	J21	·E.1	555	55.501					
2110										

Table 4	_	-	the	coor	dina	tes	of t	he C	YP3A	mod	el					
HEADER		P3A7				2011		^ ~								
TITLE		DEL OF														
AUTHOR		LOISE													mun	
SEQRES	1	459		PHE												
SEQRES	2	459		THR												
SEQRES	3	459		TRP												
SEQRES	4	459		THR												
SEQRES	5	459		CYS												
SEQRES	6	459		VAL												
SEQRES	7	459	ASP	GLU	GLU	TRP	LYS	ARG	ILE	ARG	SER	LEU	LEU	SER	PRO	
SEQRES	8	459	THR	PHE	THR	SER	GLY	LYS	LEU	LYS	GLU	MET	VAL	PRO	ILE	
SEQRES	9	459	ILE	ALA	GLN	TYR	GLY	ASP	VAL	LEU	VAL	ARG	ASN	LEU	ARG	
SEQRES	10	459	ARG	GLU	ALA	GLU	THR	GLY	LYS	PRO	VAL	THR	LEU	LYS	HIS	
SEQRES	11	459		PHE												
SEQRES	12	459	SER	PHE	GLY	VAL	SER	ILE	ASP	SER	LEU	ASN	ASN	PRO	GLN	
SEQRES	13	459		PRO												
SEQRES	14	459		PRO												
SEQRES	15	459		PHE												
SEQRES	16	459		PHE												
	17	459		LYS												
SEQRES				HIS												
SEQRES	18	459														
SEQRES	19	459		ASN												
SEQRES	20	459		LEU												
SEQRES	21	459		GLY												
SEQRES	22	459		TYR												
SEQRES	23	459		GLN												
SEQRES	24	459		PRO												
SEQRES	25	459		MET												
SEQRES	26	459	ALA	MET	ARG	LEU	GLU	ARG	VAL	CYS	LYS	LYS	ASP	VAL	GLU	
SEQRES	27	459	ILE	ASN	GLY	MET	PHE	ILE	PRO	LYS	GLY	VAL	VAL	VAL	MET	
SEQRES	28	459	ILE	PRO	SER	TYR	VAL	LEU	HIS	HIS	ASP	PRO	LYS	TYR	TRP	
SEQRES	29	459	THR	GLU	PRO	GLU	LYS	PHE	LEU	PRO	GLU	ARG	PHE	SER	LYS	
SEQRES	30	459	LYS	ASN	LYS	ASP	ASN	ILE	ASP	PRO	TYR	ILE	TYR	THR	PRO	
SEQRES	31	459		GLY												
SEQRES	32	459		LEU												
SEQRES	33	459		ASN												
SEQRES	34	459		LEU												
SEQRES	35	459		PRO												
SEQRES	36	459		SER				D 13	nun	ODO	, OLI			-		
HET	HEM	600		JLK	GHI	ADA										
		HEM														
HETNAM				7 - 7 5	TD AM	FTUV	T _ O	13-5	TUTN	VT _2	10_	DOD D	UTNE	מם זחי	OPIONIC	ACID
HETSYN							ъ-о,	13-5	T A T !!	111-2	, 10-	FORF	HIME	DIEN	OFTONIC	ACID
FORMUL			H34		4 FE		760	_	244	_ c	. 895	1	00	0.00	ı	3A7
ATOM	1		PRO	45			.768		.244							3A7
MOTA	2		PRO	45			.053		.448		.648		00	0.00		
MOTA	3		PRO	45			.705		.319		.064		00	0.00		3A7
MOTA	4		PRO	45			.467		.950		.422		00	0.00		3A7
ATOM	5	CG	PRO	45			.292		.018		.139		00	0.00		3A7
MOTA	6	С	PRO	45			.594		.801		7.950		00	0.00		3A7
ATOM	7	0	PRO	45		23	.387		.010		3.057		00	0.00		3A7
ATOM	8	N	PHE	46			.870		.857		3.600		00	0.00		3A7
MOTA	9	CA	PHE	46		21	.751	. 5	.140	9	9.472	1.	00	0.00		3A7
ATOM	10	CB	PHE	46		21	.853	4	.416	-10	0.835	1.	00	0.00)	3A7
ATOM	11	CG	PHE	46		23	.083	4	.887	-13	1.553	3 1.	.00	0.00)	3A7
ATOM	12	CD1	PHE	46		24	.173	4	.033	-13	1.730) 1.	.00	0.00)	3A7
ATOM	13	CD2	PHE	46		23	.155	• 6	.189	-12	2.049	1.	.00	0.00)	3A7
ATOM	14	CE1		46			.317		.474	-13	2.390	1.	.00	0.00)	3A7
ATOM	15	CE2		46			.297				2.709		.00	0.00)	3A7
ATOM	16	CZ	PHE	46			.380				2.879		.00	0.00		3A7
ATOM	17	Č	PHE	46			. 491		. 691		8.782		.00	0.00		3A7
ATOM	18	ŏ	PHE	46			. 400		.166		9.096		.00	0.0		3A7
ATOM	19	Ŋ	LEU	47			629		3.749		7.81		.00	0.0		3A7
ATOM	20	CA		47			0.541		3.204		7.03		.00	0.0		3A7
			LEU				9.661				6.87		.00	0.0		3A7
ATOM	21	CB	LEU	47					1.667				.00	0.0		3A7
ATOM	22	CG	LEU	47			3.490).978		6.129			0.0		3A7
ATOM	23	CD1		47			1.133		1.202		6.82		.00			
ATOM	24	CD2		47			3.768		.526		5.94		.00	0.0		3A7
ATOM	25	C	LEU	47			5.573		3.860		5.68		.00	0.0		3A7
ATOM	26	0	LEU	47			0.619		3.930		5.03		.00	0.0		3A7
MOTA	27	N	GLY	48			3.396		1.349		5.22		.00	0.0		3A7
ATOM	28	CA	GLY	48		18	3.240) 4	4.96	5 -	3.93	3 I	.00	0.0	U	3A7

ATOM	29	С	GLY	48	16.930	4.491	-3.395	_	0.00	3A7
ATOM	30	0	GLY	48	15.938	5.218	-3.414		0.00 0.00	3A7 3A7
ATOM	31	N	ASN	49 49	16.911 15.741	3.229 2.585	-2.898 -2.348	1.00	0.00	3A7
ATOM ATOM	32 33	CA CB	ASN ASN	49	15.445	1.235	-3.059	1.00	0.00	3A7
ATOM	34	CG	ASN	49	14.046	0.705	-2.706	1.00	0.00	3A7
ATOM	35		ASN	49	13.035	1.349	-3.011	1.00	0.00	3A7
ATOM	36	ND2		49	14.005	-0.494	-2.051	1.00	0.00	3A7
MOTA	37	C	ASN	49	16.016	2.375	-0.880	1.00	0.00	3A7 3A7
ATOM	38 39	O N	ASN ALA	49 50	17.169 14.933	2.278 2.293	-0.463 -0.065	1.00	0.00	3A7
ATOM ATOM	40	CA	ALΛ	50	14.998	2.111	1.369	1.00	0.00	3A7
ATOM	41	СВ	ALA	50	13.847	2.834	2.098	1.00	0.00	3A7
MOTA	42	С	ALA	50	14.941	0.641	1.697	1.00	0.00	3A7
ATOM	43	0	ALA	50	13.866	0.049	1.787	1.00	0.00	3A7 3A7
ATOM	44	N	LEU	51	16.133	0.032 -1.360	1.885 2.232	1.00 1.00	0.00	3A7
ATOM ATOM	45 46	CA CB	LEU LEU	51 51	16.271 16.271	-2.314	1.001	1.00	0.00	3A7
ATOM	47	CG	LEU	51	17.055	-1.862	-0.262	1.00	0.00	3A7
ATOM	48		LEU	51	18.587	-1.811	-0.098	1.00	0.00	3A7
ATOM	49	CD2	LEU	· 51	16.690	-2.765	-1.456	1.00	0.00	3A7
ATOM	50	С	LEU	51	17.550	-1.468	3.012	1.00	0.00	3A7 3A7
ATOM	51	0	LEU	51 52	18.327 17.794	-0.517 -2.657	3.085 3.613	1.00	0.00	3A7
ATOM ATOM	52 53	N CA	SER SER	52 52	19.005	-2.956	4.343	1.00	0.00	3A7
ATOM	54	CB	SER	52	18.741	-3.361	5.821	1.00	0.00	3A7
ATOM	55	OG	SER	52	17.737	-4.363	5.945	1.00	0.00	3A7
MOTA	56	С	SER	52	19.734	-4.023	3.562	1.00	0.00	3A7
ATOM	57	0	SER	52	20.164	-3.782	2.435	1.00	0.00	3A7 3A7
ATOM	58	N	PHE	53 53	19.898 20.599	-5.231 -6.341	4.155 3.550	1.00	0.00	3A7
ATOM ATOM	59 60	CA CB	PHE	53 53	21.908	-6.703	4.297	1.00	0.00	3A7
ATOM	61	CG	PHE	53	22.730	-5.456	4.439	1.00	0.00	3A7
ATOM	62	CD1	PHE	53	22.819	-4.809	5.673	1.00	0.00	3A7
ATOM	63		PHE	53	23.346	-4.880	3.327	1.00	0.00	3A7
ATOM	64		PHE	53	23.491	3.598	5.793	1.00	0.00	3A7 3A7
ATOM ATOM	65 66	CEZ	PHE PHE	53 53	24.018 24.085	-3.667 -3.022	3.446 4.675	1.00	0.00	3A7
ATOM	67	c	PHE	53	19.639	-7.494	3.594	1.00	0.00	3A7
ATOM	68	0	PHE	53	19.885	-8.495	4.264	1.00	0.00	3A7
ATOM	69	N	ARG	54	18.491	-7.330	2.875	1.00	0.00	3A7
MOTA	70	CA	ARG	54	17.327	-8.205	2.828	1.00	0.00	3A7 3A7
ATOM	71 72	CB CG	ARG ARG	54 54	17.629	-9.719 -10.045	2.641 1.437	1.00	0.00	3A7
ATOM ATOM	73	CD	ARG	54	17.996	-9.573	0.079	1.00	0.00	3A7
ATOM	74	NE	ARG	54	19.049	-9.836	-0.962	1.00	0.00	3A7
ATOM	75	CZ	ARG	54		-10.925	-1.791	1.00	0.00	3A7
ATOM	76		LARG	54		-11.113	-2.669	1.00	0.00	3A7 3A7
ATOM	77 78	NH2	2 ARG	54 54	18.013 16.514	-11.826 -7.983	-1.753 4.087	1.00	0.00	3A7
ATOM ATOM	70 79	o	ARG ARG	54	16.760	-8.611	5.116	1.00	0.00	3A7
ATOM	80	N	LYS	55	15.545	-7.030		1.00	0.00	3A7
MOTA	81	CA	LYS	55	14.927	-6.447	5.205		0.00	3A7
ATOM	82	CB	LYS	55	14.520	-4.971	5.023		0.00	3A7 3A7
ATOM	83	CG	LYS	55	13.327 13.574	-4.656 -4.842			0.00	3A7
ATOM ATOM	84 85	CD		55 55	13.074	-6.171				3A7
ATOM	86		LYS	55	11.612	-6.322				3A7
ATOM	87		LYS	55	13.767	-7.241				3A7
MOTA	88		LYS	55	13.403	-7.067				3A7
ATOM	89		GLY	56 56	13.158	-8.146				3A7 3A7
ATOM ATOM	90 91		GLY GLY	56 56	12.066	-8.950 -10.146				3A7
ATOM	92		GLY	56		-10.334				3A7
ATOM	93		TYR			-11.031				3A7
ATOM	94				13.171	-12.222	3.922			3A7
MOTA	95					-12.913				3A7
ATOM	96					-13.558				3A7 3A7
ATOM ATOM	97 98		1 TYR 2 TYR			-12.832 -14.898				3A7
MOTA	99		1 TYR			-13.440				3A7
ATOM	100		2 TYR			-15.506				3A7

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ATOM	101	CZ	TYR	57	16.538 -	-14.777	1.021	1.00	0.00	3A7
MOTA	102	ОН	TYR	57	17.229 -	-15.392	-0.043	1.00	0.00	3A7
MOTA	103	C	TYR	57	12.013 -	-13.191	4.022	1.00	0.00	3A7
MOTA	104	0	TYR	57	11.631 -		3.021	1.00	0.00	3A7
MOTA	105	N	TRP	58	11.379 -		5.211	1.00	0.00	3A7
ATOM	106	CA	TRP	58	10.261 -		5.359	1.00	0.00	3A7 3A7
ATOM	107	CB	TRP	58 50	9.872 -		6.832	1.00	0.00	3A7
ATOM ATOM	108 109	CG	TRP TRP	58 58		-13.318 -13.247	7.606 8.157	1.00	0.00	3A7
ATOM	110		TRP	58		-12.115	7.871	1.00	0.00	3A7
ATOM	111		TRP	58		-11.297	8.548	1.00	0.00	3A7
ATOM	112		TRP	58		-11.978	8.741	1.00	0.00	3A7
ATOM	113		TRP	58	6.969	-14.158	8.175	1.00	0.00	3A7
ATOM	114	CZ2	TRP	58	6.694	-11.604	9.360	1.00	0.00	3A7
ATOM	115		TRP	58		-13.780	8.796	1.00	0.00	3A7
ATOM	116		TRP	58		-12.522	9.382	1.00	0.00	3A7
ATOM	117	Ç	TRP	58		-13.824	4.612	1.00	0.00	3A7 3A7
ATOM	118	0	TRP	58 59		-14.664 -12.490	4.106 4.502	1.00 1.00	0.00	3A7
ATOM ATOM	119 120	N CA	THR THR	59 59		-12.490	3.737	1.00	0.00	3A7
ATOM	121	CB	THR	59		-10.582	4.136	1.00	0.00	3A7
ATOM	122		THR	59	8.282	-9.643	4.073	1.00	0.00	3 A 7
ATOM	123		THR	59		-10.634	5.579	1.00	0.00	3A7
ATOM	124	C	THR	59	7.925	-12.067	2.267	1.00	0.00	3A7
ATOM	125	0	THR	59	7.011	-12.232	1.471	1.00	0.00	3A7
ATOM	126	N	PHE	60		-12.018	1.884	1.00	0.00	3A7
ATOM	127	CA	PHE	60		-12.244	0.530	1.00	0.00	3A7
ATOM	128	СВ	PHE	60	11.132		0.330	1.00	0.00	3A7 3A7
ATOM	129	CG	PHE	60 60		-11.735 -10.822	-1.126 -1.978	1.00	0.00	3A7
ATOM ATOM	130 131		PHE	60 60		-10.822	-1.647	1.00	0.00	3A7
ATOM	132		PHE	60		-10.772	-3.328	1.00	0.00	3A7
ATOM	133		PHE	60		-12.548	-2.997	1.00	0.00	3A7
ATOM	134	CZ	PHE	60	12.186	-11.636	-3.839	1.00	0.00	3A7
ATOM	135	С	PHE	60	9.505	-13.695	0.122	1.00	0.00	3A7
MOTA	136	0	PHE	60		-14.011	-0.936	1.00	0.00	3A7
MOTA	137	N	ASP	61		-14.632	0.991	1.00	0.00	3A7
MOTA	138	CA	ASP	61		~16.051	0.737	1.00	0.00 0.00	3A7 3A7
ATOM	139 140	CB CG	ASP ASP	61 61		-16.892 -16.729	1.774	1.00	0.00	3A7
ATOM ATOM	141		ASP	61		-16.736	0.447	1.00	0.00	3A7
ATOM	142		ASP	61		-16.555	2.655	1.00	0.00	3A7
ATOM	143	Ċ	ASP	61		-16.503	0.698	1.00	0.00	3A7
MOTA	144	0	ASP	61	8.070	-17.371	-0.085	1.00	0.00	3A7
MOTA	145	N	MET	62		-15.870	1.491	1.00	0.00	3A7
ATOM	146	CA	MET	62		-16.134	1.452	1.00	0.00	3A7
ATOM	147	CB	MET	62		-15.468	2.623	1.00	0.00	3A7 3A7
ATOM ATOM	148 149	CG	MET MET	62 62		-16.224 -15.359	3.947 5.422	1.00	0.00	3A7
ATOM	150	CE	MET	62		-15.481	5.031	1.00	0.00	3A7
ATOM	151	c	MET	62		-15.672	0.168	1.00	0.00	3A7
ATOM	152	Ō	MET	62		-16.335	-0.342	1.00	0.00	3A7
ATOM	153	N	GLU	63	5.922	-14.555	-0.430	1.00	0.00	3A7
ATOM	154	CA	GLU	63		-14.094	-1.722	1.00	0.00	3A7
MOTA	155	СВ	GLU	63		-12.683	-2.039	1.00	0.00	3A7
MOTA	156	CG	GLU	63		-11.593	-1.206	1.00	0.00	3A7
ATOM	157	CD	GLU	63		-10.239 -10.169	-1.427 -2.214	1.00	0.00	3A7 3A7
ATOM ATOM	158 159		GLU GLU	63 63	5.495	-9.249	-0.802	1.00	0.00	3A7
ATOM	160	C	GLU	63		-15.044	-2.831	1.00	0.00	3A7
ATOM	161	ŏ	GLU	63		-15.339	-3.734	1.00	0.00	3A7
ATOM	162	N	CYS	64		-15.606	-2.747		0.00	3A7
ATOM	163	CA	CYS	64		-16.598	-3.674		0.00	3A7
ATOM	164	CB	CY\$	64		-16.969	-3.362		0.00	3A7
MOTA	165	SG	CYS	64		-15.524	-3.736		0.00	3A7
ATOM	166	C	CYS	64		-17.853	-3.631		0.00	3A7
ATOM	167	0	CYS	64 65		-18.402	-4.655		0.00	3A7 3A7
ATOM ATOM	168 169	N CA	TYR TYR	65 65		-18.323 -19.526	-2.413 -2.251			3A7
ATOM	170	CB	TYR			-19.993	-0.802			3A7
ATOM	171	CG	TYR			-20.246	-0.379			3A7
ATOM	172		I TYR			-19.725	0.834			3A7

ATOM	173	CD2	TYR	65	7.985 -	-20.850	-1.222	1.00	0.00	3A7
ATOM	174	CE1		65	8.800 -	-19.750	1.182	1.00	0.00	3A7
ATOM	175	CE2	TYR	65	9.336 -	-20.816	-0.901	1.00	0.00	3A7 ·
ATOM	176	CZ	TYR	65		-20.216	0.283	1.00	0.00	3A7
ATOM	177	ОН	TYR	65	11.101		0.572	1.00	0.00	3A7
MOTA	178	C	TYR	65		-19.373	-2.701	1.00	0.00	3A7
ATOM	179	0	TYR	65 66		-20.319	-3.228 -2.556	1.00	0.00	3A7 3A7
ATOM	180 181	N CA	LYS LYS	66 66		-18.174 -17.922	-3.043	1.00	0.00	3A7
ATOM ATOM	182	CB	LYS	66		-16.564	-2.544	1.00	0.00	3A7
ATOM	183	CG	LYS	66		-16.579	-1.049	1.00	0.00	3A7
ATOM	184	CD	LYS	66		-15.185	-0.470	1.00	0.00	3A7
MOTA	185	CE	LYS	66	-0.063	-14.502	-1.089	1.00	0.00	3A7
ATOM	186	NZ	LYS	66	-0.299		-0.461	1.00	0.00	3A7
MOTA	187	С	LYS	66		-17.957	-4.556	1.00	0.00	3A7
ATOM	188	0	LYS	66		-18.326	-5.129	1.00	0.00	3A7
ATOM	189	N	LYS	67		-17.595	-5.243	1.00	0.00	3A7 3A7
ATOM	190	CA	LYS	67 67		-17.539 -16.414	-6.682 -7.137	1.00	0.00	3A7
MOTA MOTA	191 192	CB CG	LYS LYS	67		-16.145	-8.651	1.00	0.00	3A7
ATOM	193	CD	LYS	67		-14.878	-9.034	1.00	0.00	3A7
ATOM	194	CE	LYS	67		-14.629		1.00	0.00	3A7
ATOM	195	NZ	LYS	67		-14.424		1.00	0.00	3A7
ATOM	196	C	LYS	67	3.853	-18.855	-7.284	1.00	0.00	3A7
ATOM	197	0	LYS	67		-19.336	-8.244	1.00	0.00	3A7
MOTA	198	N	TYR	68		-19.451	-6.748	1.00	0.00	3A7
ATOM	199	CA	TYR	68		-20.573	-7.355	1.00	0.00	3A7
ATOM	200	CB	TYR	68		-20.402	-7.314	1.00	0.00	3A7 3A7
ATOM	201 202	CG	TYR TYR	68 68		-19.259 -17.989	-8.216 -7.702	1.00	0.00	3A7
ATOM ATOM	202		TYR	68		-19.457	-9.595	1.00	0.00	3A7
ATOM	204		TYR	68		-16.937	-8.550	1.00	0.00	3A7
ATOM	205		TYR	68		-18.408		1.00	0.00	3A7
ATOM	206	CZ	TYR	68	8.193	-17.146	-9.924	1.00	0.00	3A7
ATOM	207	OH	TYR	68		-16.080		1.00	0.00	3A7
ATOM	208	С	TYR	68		-21.899	-6.770	1.00	0.00	. 3A7
ATOM	209	0	TYR	68		-22.918	-7.453	1.00	0.00	3A7
ATOM	210	N	ARG	69		-21.912	-5.500	1.00	0.00	3A7 3A7
ATOM ATOM	211 212	CA CB	ARG ARG	69 69		-23.040 -23.733	-4.856 -5.717	1.00	0.00	3A7
ATOM	213	CG	ARG	69		-22.762	-6.180	1.00	0.00	3A7
ATOM	214	CD	ARG	69		-23.441	-7.009	1.00	0.00	3A7
ATOM	215	NE	ARG	69		-23.933	-8.287	1.00	0.00	3A7
MOTA	216	CZ	ARG	69	0.741	-24.664	-9.197	1.00	0.00	3A7
ATOM	217		ARG	69		-25.083		1.00	0.00	3A7
ATOM	218		ARG	69		-24.981	-8.963	1.00	0.00	3A7
MOTA	219	C	ARG	69		-23.968	-4.257	1.00	0.00	3A7 3A7
ATOM ATOM	220 221	0	ARG LYS	69 70		-23.556 -25.251	-3.663 -4.585	1.00	0.00	3A7
ATOM	222	N CA	LYS	70		-26.459	-4.410	1.00	0.00	3A7
ATOM	223	СВ	LYS	70		-27.726	-4.955	1.00	0.00	3A7
ATOM	224	CG	LYS	70		-28.142	-4.233	1.00	0.00	3A7
ATOM	225	CD	LYS	70		-27.345	-4.536	1.00	0.00	3A7
ATOM	226	CE	LYS	70		-27.577	-5.929	1.00	0.00	3A7
MOTA	227	NZ	LYS	70		-26.976	-7.009	1.00	0.00	3A7
ATOM	228	C	LYS	70		-26.352	-5.122	1.00	0.00	3A7
ATOM	229	0	LYS	70 71		-26.860 -25.662	-6.233 -4.449	1.00	0.00	3A7 3A7
ATOM ATOM	230 231	N CA	VAL VAL	71 71		-25.641	-4.770	1.00	0.00	3A7
ATOM	232	CB	VAL	71		-26.967	-5.362	1.00	0.00	3A7
ATOM	233		. VAL	71		-26.882	-5.635	1.00	0.00	3A7
ATOM	234		VAL	71		-28.158	-4.411	1.00	0.00	3A7
MOTA	235	C	VAL	71		-24.472	-5.708	1.00	0.00	3A7
MOTA	236	0	VAL	71		-24.376		1.00	0.00	3A7
ATOM	237	N	TRP	72		-23.545	-5.337		0.00	3A7
MOTA	238	CA	TRP	72		-22.433		1.00	0.00	3A7
ATOM	239	CB	TRP	72 72		-21.089 -19.873			0.00	3A7 3A7
MOTA MOTA	240 241	CDS	TRP TRP	72 72		-19.673			0.00	3A7
ATOM	242		TRP	72		-19.633			0.00	3A7
ATOM	243		TRP	72		-18.438			0.00	3A7
MOTA	244		TRP	72		-17.866				3A7

ATOM	245	CE3	TRP	72	10.923	-18.434	-7.436	1.00	0.00	3A7
MOTA	246	CZ2	TRP	72	12.368	-16.672	-5.760	1.00	0.00	3A7
ATOM	247	CZ3		72	11.414		-7.920	1.00	0.00	3A7
ATOM	248	CH2		72	12.124		-7.094	1.00	0.00	3A7
ATOM	249	С	TRP	72	12.229		-6.064	1.00	0.00	3A7
ATOM	250	0	TRP	72	12.824		-5.112	1.00	0.00	3A7
MOTA	251	N	GLY	73	12.861	-21.582	-7.022	1.00	0.00	3A7
ATOM	252	CA	GLY	73	14.278	-21.323	-6.985	1.00	0.00	3A7
ATOM	253	С	GLY	73	14.511	-19.850	-6.821	1.00	0.00	3A7
ATOM	254	ō	GLY	73	13.812		-7.409	1.00	0.00	3A7
ATOM	255	N	ILE	74	15.530		-6.009	1.00	0.00	3A7
ATOM	256	CA	ILE	74	15.929		-5.754	1.00	0.00	3A7
ATOM	257	CB	ILE	74	15.600	-17.676	-4.328	1.00	0.00	3A7
MOTA	258	CG2	ILE	74	16.301	~18.543	-3.258	1.00	0.00	3A7
ATOM	259	CG1	ILE	74	15.835	-16.159	-4.124	1.00	0.00	3A7
ATOM	260	ÇD	ILE	74	15.205		-2.836	1.00	0.00	3A7
ATOM	261	Ċ	ILE	74	17.407		-6.023	1.00	0.00	3A7
ATOM	262	0	ILE	74	18.100		-5.904	1.00	0.00	3A7
ATOM	263	N	TYR	75	17.928	-16.900	-6.425	1.00	0.00	3A7
MOTA	264	CA	TYR	75	19.303	-16.765	-6.827	1.00	0.00	3A7
MOTA	265	СВ	TYR	75	19.424	-16.348	-8.308	1.00	0.00	3A7
ATOM	266	CG	TYR	75	18.811	-17.400	-9.184	1.00	0.00	3A7
ATOM	267		TYR	75	17.487		-9.613	1.00	0.00	3A7
ATOM	268		TYR	75	19.554		-9.582	1.00	0.00	3A7
ATOM	269		TYR	75		-18.261		1.00	0.00	3A7
ATOM	270	CE2	TYR	75	18.983	-19.489	-10.394	1.00	0.00	3A7
ATOM	271	CZ	TYR	75	17.660	-19.367	-10.807	1.00	0.00	3A7
MOTA	272	ОН	TYR	75	17.079	-20.361	-11.624	1.00	0.00	3A7
ATOM	273	C	TYR	75		-15.716	-5.954	1.00	0.00	3A7
ATOM	274	ŏ	TYR	75		-14.543	-6.059	1.00	0.00	3A7
MOTA	275	N	ASP	76		-16.106	-5.059	1.00	0.00	3A7
ATOM	276	CA	ASP	76	21.559	-15.171	-4.194	1.00	0.00	3A7
MOTA	277	CB	ASP	76	21.470	-15.513	-2.685	1.00	0.00	3A7
ATOM	278	CG	ASP	76	20.053	-15.259	-2.172	1.00	0.00	3A7
ATOM	279	OD1	ASP	76	19,105	-15.935	-2.652	1.00	0.00	3A7
ATOM	280		ASP	76		-14.382	-1.279	1.00	0.00	3A7
ATOM	281	c	ASP	76		-15.175	-4.597	1.00	0.00	3A7
ATOM	282	0	ASP	76		-16.000	-4.149	1.00	0.00	3A7
MOTA	283	N	CYS	77		-14.210	-5.459	1.00	0.00	3A7
ATOM	284	CA	CYS	77	24.738	-13.896	-5.902	1.00	0.00	3 A 7
ATOM	285	CB	CYS	77	25.569	-13.074	-4.858	1.00	0.00	3A7
ATOM	286	SG	CYS	77	25.906	-13.854	-3.237	1.00	0.00	3A7
ATOM	287	С	CYS	77		-15.056	-6.442	1.00	0.00	3A7
ATOM	288	ŏ	CYS	77		-15.442	-5.879	1.00	0.00	3A7
ATOM	289	N	GLN	78		-15.613	-7.583	1.00	0.00	3A7
MOTA	290	CA	GLN	78		-16.622	-8.369	1.00	0.00	3A7
ATOM	291	СВ	GLN	78	27.325	-16.549	-8.440	1.00	0.00	3A7
ATOM	292	CG	GLN	78	27.848	-15.222	-9.017	1.00	0.00	3A7
MOTA	293	CD	GLN	78	29.378	-15.274	-9.063	1.00	0.00	3A7
ATOM	294		GLN	78		-16.057	-9.823	1.00	0.00	3A7
ATOM	295		GLN	78		-14.415	-8.222	1.00	0.00	3A7
ATOM	296	С	GLN	78		-18.037	-8.023	1.00	0.00	3A7
ATOM	297	0	GLN	78		-18.949	-8.771	1.00	0.00	3A7
MOTA	298	N	GLN	79		-18.277	-6.903	1.00	0.00	3A7
ATOM	299	CA	GLN	79	24.270	-19.620	-6.516	1.00	0.00	3A7
ATOM	300	СВ	GLN	79		-19.978	-5.085	1.00	0.00	3A7
ATOM	301	CG	GLN	79		-19.895	-4.897	1.00	0.00	3A7
ATOM	302	CD	GLN	79		-20.276		1.00	0.00	3A7
ATOM	303		GLN	79		-19.589		1.00	0.00	3A7
ATOM	304		GLN	79		-21.399		1.00	0.00	3A7
ATOM	305	С	GLN	79	22.765	-19.774	-6.615	1.00	0.00	3A7
ATOM	306	0	GLN	79	22.037	-18.847	-6.260	1.00	0.00	3A7
ATOM	307	N	PRO	80	22.241	-20.926	-7.069	1.00	0.00	3A7
ATOM	308	CA	PRO	80		-21.225		1.00	0.00	3A7
ATOM	309	CD	PRO	80		-21.867	-7.907	1.00	0.00	3A7
ATOM	310	СВ	PRO	80		-22.191	-8.214	1.00	0.00	3A7
ATOM	311	CG	PRO	80		-22.915		1.00	0.00	3A7
MOTA	312	С	PRO	80		-21.899		1.00	0.00	3A7
MOTA	313	0	PRO	80	21.269	-22.746	-5.277	1.00	0.00	3A7
ATOM	314	N	MET	81	19.342	-21.571	-5.140	1.00	0.00	3A7
ATOM	315	CA	MET	81		-22.233		1.00	0.00	3A7
ATOM	316	СВ	MET	81		-21.392		1.00	0.00	3A7
	510	U		.	17.070	-1.332	2.005	1.00	5.00	JAI

ATOM	317	CG	MET	81	20.582	-21.043	-2.428	1.00	0.00	3A7
ATOM	318	SD	MET	81	20.947	-20.209	-0.854	1.00	0.00	3A7
ATOM	319	CE	MET	81	20.120		-1.276	1.00	0.00	3A7
MOTA	320	C	MET	81	17.447		-4.177	1.00	0.00	3A7
ATOM	321	0	MET	81	16.677		-4.447	1.00	0.00	3A7
ATOM	322	И	LEU	82	17.035		-4.052	1.00	0.00	3A7 3A7
ATOM	323	CA	LEU	82 82	15.657 15.468		-4.201 -4.990	1.00	0.00	3A7
ATOM ATOM	324 325	CB CG	LEU LEU	82 82	15.574		-6.509	1.00	0.00	3A7
ATOM	326		LEO .	82	16.903		-7.137	1.00	0.00	3A7
ATOM	327		LEU	82	14.352		-7.300	1.00	0.00	3A7
ATOM	328	C	LEU	82	15.022		-2.843	1.00	0.00	3A7
ATOM	329	0	LEU	82	15.439	-24.903	-1.947	1.00	0.00	3A7
ATOM	330	N	ALA	83	13.975	-23.351	-2.673	1.00	0.00	3A7
MOTA	331	CA	ALA	83	13.243		-1.443	1.00	0.00	3A7
ATOM	332	CB	ALA	83	12.731		-1.267	1.00	0.00	3A7
ATOM	333	С	ALA	83		-24.096	-1.430	1.00	0.00	3A7
MOTA	334	0	ALA	83	11.193		-2.320	1.00	0.00	3A7 3A7
MOTA MOTA	335 336	N CA	ILE	84 84	11.963 10.949		-0.399 -0.290	1.00	0.00	3A7
ATOM	337	CB	ILE	84	11.517		0.009	1.00	0.00	3A7
MOTA	338		ILE	84		-28.307	0.374	1.00	0.00	3A7
ATOM	339		ILE	84		-28.016	-1.243	1.00	0.00	3A7
ATOM	340	CD	ILE	84	13.207	-27.201	-2.013	1.00	0.00	3A7
MOTA	341	С	ILE	84	10.004	-25.576	0.802	1.00	0.00	3A7
ATOM	342	0	ILE	84		-25.289	1.921	1.00	0.00	3A7
MOTA	343	N	THR	85		-25.597	0.509	1.00	0.00	3A7
ATOM	344	CA	THR	85		-25.139	1.413	1.00	0.00	3A7
ATOM	345	CB	THR	85		-23.819	0.999	1.00	0.00	3A7
ATOM	346		THR	85		-23.627 -22.782	-0.412 1.725	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	347 348	C	THR THR	85 85		-26.125	1.486	1.00	0.00	3A7
ATOM	349	ŏ	THR	85		-26.730	0.619	1.00	0.00	3A7
ATOM	350	N	ASP	86		-26.396	2.502	1.00	0.00	3A7
ATOM	351	CA	ASP	86		-27.263	2.510	1.00	0.00	3A7
ATOM	352	СВ	ASP	86	3.722	-27.421	1.361	1.00	0.00	3A7
ATOM	353	CG	ASP	86		-26.055	0.952	1.00	0.00	3A7
MOTA	354		ASP	86		-25.362	1.833	1.00	0.00	3A7
ATOM	355		ASP	86		-25.692	-0.246	1.00	0.00	3A7
ATOM	356	C	ASP	86		-28.602	3.011	1.00	0.00	3A7 3A7
ATOM ATOM	357 358	O N	ASP PRO	86 87		-28.994 -29.324	2.738 3.756	1.00	0.00	3A7
ATOM	359	CA	PRO	87		-30.519	4.472	1.00	0.00	3A7
ATOM	360	CD	PRO	87		-28.734	4.388	1.00	0.00	3A7
ATOM	361	СВ	PRO	87		-30.942	5.276	1.00	0.00	3A7
ATOM	362	CG	PRO	87	2.505	-29.914	4.977	1.00	0.00	3A7
MOTA	363	С	PRO	87	5.202	-31.641	3.571	1.00	0.00	3A7
MOTA	364	0	PRO	87		-32.375	3.920	1.00	0.00	3A7
ATOM	365	N	ASP.	88		-31.800	2.413	1.00	0.00	3A7 .
MOTA	366 367	CA CB	ASP	88		-32.846 -32.701	1.455 0.270	1.00	0.00	3A7 3A7
ATOM ATOM	368	CG	ASP ASP	88 88		-32.701	0.749	1.00	0.00	3A7
MOTA	369		ASP	88		-33.640	1.676	1.00	0.00	3A7
ATOM	370		ASP	88		-32.094	0.198	1.00	0.00	3A7
ATOM	371	С	ASP	88		-32.787	0.909	1.00	0.00	3A7
ATOM	372	0	ASP	88	6.874	-33.798	0.830	1.00	0.00	3A7
MOTA	373	N	MET	. 89		-31.588	0.554	1.00	0.00	3A7
ATOM	374	CA	MET	89		-31.388	0.009	1.00	0.00	3A7
MOTA	375	СВ	MET	89		-30.073	-0.773	1.00	0.00	3A7
MOTA	376	CG	MET	89		-30.035	-1.918	1.00	0.00	3A7 3A7
ATOM	377	SD	MET	89		-28.663 -27.425	-1.731 -1.755	1.00	0.00	3A7
ATOM ATOM	378 379	CE	MET MET	89 89		-31.390	1.081	1.00	0.00	3A7
ATOM	380	Ö	MET	89		-31.936	0.893	1.00		3A7
ATOM	381	N	ILE	90		-30.824	2.267	1.00		3A7
ATOM	382	CA	ILE	90		-30.812	3.398	1.00		3A7
ATOM	383	СВ	ILE	90		-29.908	4.501	1.00		3A7
MOTA	384		ILE	90		-30.036		1.00		3A7
MOTA	385		ILE	90		-28.467	3.973	1.00		3A7
ATOM	386	CD	ILE	90		-27.853		1.00		3A7 3A7
ATOM ATOM	387	C O	ILE	90 90		-32.218 -32.588		1.00		3A7 3A7
ATOM	388	J	ILE	50	11.016	-32.300	7.440	1.00	0.00	JAI

ATOM	389	N	LYS	91	8.877 -	-33.100	3.925	1.00	0.00	3A7
MOTA	390	CA	LYS	91	9.058 -		4.328	1.00	0.00	3A7
ATOM	391	CB	LYS	91	7.722 -		4.361	1.00	0.00	3A7
ATOM	392	CG	LYS	91	7.790 -		5.036 5.192	1.00	0.00	3A7 3A7
ATOM ATOM	393 394	CE	LYS LYS	91 91	6.407 - 6.465 -		5.898	1.00	0.00	3A7
ATOM	395	NZ	LYS	91	5.108 -		6.031	1.00	0.00	3A7
ATOM	396	C	LYS	91	10.010		3.414	1.00	0.00	3A7
MOTA	397	0	LYS	91	10.824	-36.021	3.838	1.00	0.00	3A7
MOTA	398	N	THR	92		-34.861	2.113	1.00	0.00	3A7
MOTA	399	CA	THR	92	10.864		1.113	1.00	0.00	3A7
ATOM	400	CB	THR	92	10.441		-0.272 -0.430	1.00	0.00	3A7 3A7
ATOM ATOM	401 402		THR THR	92 92	11.180	-35.206 -35.836	-1.323	1.00	0.00	3A7
ATOM	403	C	THR	92	12.263		1.326	1.00	0.00	3A7
ATOM	404	ō	THR	92	13.222		1.196	1.00	0.00	3A7
ATOM	405	N	VAL	93	12.395		1.730	1.00	0.00	3A7
MOTA	406	CA	VAL	93	13.674		1.938	1.00	0.00	3A7
ATOM	407	CB	VAL	93	13.628		2.127	1.00	0.00	3A7 3A7
ATOM	408 409		VAL VAL	93 93	12.833 13.354		1.061 3.585	1.00	0.00	3A7
MOTA MOTA	410	C	VAL	93	14.483		3.034	1.00	0.00	3A7
ATOM	411	ŏ	VAL	93	15.703		3.002	1.00	0.00	3A7
ATOM	412	N	LEU	94	13.861		3.946	1.00	0.00	3A7
MOTA	413	CA	LEU	94	14.509	-35.450	4.889	1.00	0.00	3A7
MOTA	414	СВ	LEU	94	13.538		5.429	1.00	0.00	3A7
ATOM	415	CG	LEU	94	12.454		6.397	1.00	0.00	3A7 3A7
ATOM ATOM	416 417		LEU	94 94	11.435 13.079		6.726 7.687	1.00	0.00 0.00	3A7
MOTA	418	C	LEU	94	15.673		4.325	1.00	0.00	3A7
ATOM	419	ō	LEU	94	16.786		4.842	1.00	0.00	3A7
MOTA	420	N	VAL	95	15.389	-37.041	3.249	1.00	0.00	3A7
MOTA	421	CA	VAL	95	16.254		2.446	1.00	0.00	3A7
ATOM	422	CB	VAL	95	17.146		1.449	1.00	0.00	3A7 3A7
ATOM ATOM	423 424		VAL VAL	95 95	18.293 17.667		2.088 0.379	1.00	0.00	3A7
ATOM	425	C	VAL	95		-38.932	3.269	1.00	0.00	3A7
ATOM	426	ō	VAL	95		-38.606	4.052	1.00	0.00	3A7
ATOM	427	N	LYS	96	16.651	-40.226	3.099	1.00	0.00	3A7
ATOM	428	CA	LYS	96		-41.310	3.864	1.00	0.00	3A7
ATOM	429	CB	LYS	96 06		-41.757	5.021 5.922	1.00	0.00	3A7 3A7
ATOM ATOM	430 431	CG CD	LYS LYS	96 96		-42.863 -43.296	7.055	1.00	0.00	3A7
ATOM	432	CE	LYS	96		-42.211	8.105	1.00	0.00	3A7
ATOM	433	NZ	LYS	96		-41.808	8.783	1.00	0.00	3A7
ATOM	434	С	LYS	96		-42.463	2.917	1.00	0.00	3A7
ATOM	435	0	LYS	96		-42.998	2.397	1.00	0.00	3A7 3A7
ATOM	436 437	N CA	GLU	97 97		-42.930 -42.451	2.649 3.016	1.00	0.00	3A7
ATOM ATOM	438	CB	GLU GLU	97		-41.024	2.498	1.00	0.00	. 3A7
ATOM	439	CG	GLU	97		-40.894	0.966	1.00	0.00	3A7
ATOM	440	CD	GLU	97		-41.763	0.314	1.00	0.00	3A7
MOTA	441		GLU	97		-42.695	-0.447	1.00	0.00	3A7
ATOM	442		GLU	97		-41.504	0.567	1.00	0.00	3A7 3A7
ATOM ATOM	443 444	C O	GLU GLU	97 97		-42.531 -41.560	4.499 5.238	1.00	0.00	3A7 3A7
ATOM	445	N	CYS	98		-43.711	4.956	1.00	0.00	3A7
ATOM	446	CA	CYS	98		-43.956	6.327	1.00		3A7
ATOM	447	CB	CYS	98	21.159	-45.456	6.703	1.00	0.00	3A7
ATOM	448	SG	CYS	98		-46.111	6.530	1.00		3A7
ATOM	449	C	CYS	98		-43.454	6.538	1.00		3A7
ATOM ATOM	450 451	0	CYS	98 99		-43.131 -43.358	7.656 5.423			3A7 3A7
ATOM	451 452	N CA	TYR TYR			-43.336	5.352			3A7
ATOM	453	СВ	TYR			-43.602	4.775			3A7
ATOM	454	ÇG	TYR			-44.708	5.749	1.00	0.00	3A7
MOTA	455		TYR			-45.981	5.553			3A7
ATOM	456		TYR			-44.471	6.875			3A7
ATOM	457		TYR			-47.000 -45.488	6.470 7.791			3A7 3A7
ATOM ATOM	458 459		TYR TYR			-45.488 -46.754	7.791			3A7
ATOM	460		TYR			-47.785	8.524			3A7

ATOM	461	С	TYR	99	24.459 -41.520	4.445	1.00	0.00	3A7
ATOM	462	0	TYR	99	24.717 -41.584	3.244	1.00	0.00	3A7
MOTA	463	N	SER	100	23.943 -40.407	5.029	1.00	0.00	3A7
MOTA	464	CA	SER	100	23.548 -39.211	4.317	1.00	0.00	3A7
ATOM	465	CB	SER	100	22.340 -38.501	4.990	1.00	0.00	3A7
ATOM	466	OG	SER	100	22.547 -38.275	6.381	1.00	0.00	3A7 3A7
ATOM	467	C	SER	100 100	24.721 -38.267 25.295 -37.848	4.207 5.211	1.00	0.00	3A7
ATOM ATOM	468 469	O N	SER VAL	101	25.093 -37.923	2.947	1.00	0.00	3A7
ATOM	470	CA	VAL	101	26.233 -37.096	2.616	1.00	0.00	3A7
ATOM	471	СВ	VAL	101	26.925 -37.529	1.327	1.00	0.00	3A7
ATOM	472	CG1		101	28.244 -36.746	1.143	1.00	0.00	3A7
ATOM	473	CG2	VAL	101	27.188 -39.049	1.394	1.00	0.00	3A7
ATOM	474	С	VAL	101	25.777 -35.663	2.512	1.00	0.00	3A7
ATOM	475	0	VAL	101	25.384 -35.187	1.447	1.00	0.00	3A7
ATOM	476	N	PHE	102	25.851 -34.944	3.658	1.00	0.00	3A7
ATOM	477	CA	PHE	102	25.588 -33.531	3.774	1.00 1.00	0.00	3A7 3A7
ATOM	478 479	CB	PHE	102 102	24.757 -33.208 24.515 -31.734	5.051 5.284	1.00	0.00	3A7
ATOM ATOM	480	CG	PHE	102	24.224 -30.854	4.236	1.00	0.00	3A7
ATOM	481		PHE	102	24.602 -31.227	6.582	1.00	0.00	3A7
ATOM	482		PHE	102	24.063 -29.493	4.481	1.00	0.00	3 A 7
ATOM	483		PHE	102	24.424 -29.870	6.830	1.00	0.00	3A7
ATOM	484	CZ	PHE	102	24.163 -29.000	5.777	1.00	0.00	3A7
MOTA	485	C	PHE	102	26.945 -32.887	3.838	1.00	0.00	3A7
ATOM	486	0	PHE	102	27.728 -33.174	4.741	1.00	0.00	3A7
ATOM	487	N	THR	103	27.238 -31.980	2.869	1.00	0.00	3A7
ATOM	488	CA	THR	103	28.502 -31.281	2.757 1.308	1.00 1.00	0.00	3A7 3A7
ATOM ATOM	489 490	CB OG1	THR THR	103 103	28.814 -30.904 30.168 -30.496	1.135	1.00	0.00	3A7
ATOM	491	CG2		103	27.858 -29.816	0.779	1.00	0.00	3A7
ATOM	492	C	THR	103	28.484 -30.083	3.685	1.00	0.00	3A7
ATOM	493	ō	THR	103	27.430 -29.672	4.169	1.00	0.00	3A7
ATOM	494	N	ASN	104	29.682 -29.507	3.955	1.00	0.00	3A7
MOTA	495	CA	ASN	104	29.888 -28.430	4.899	1.00	0.00	3A7
ATOM	496	CB	ASN	104	31.378 -28.320	5.343	1.00	0.00	3A7
ATOM	497	CG	ASN	104	32.353 -28.168	4.161	1.00	0.00	3A7
ATOM	498		ASN	104	32.706 -27.047	3.775	1.00	0.00	3A7 3A7
ATOM ATOM	499 500	C ND2	ASN ASN	104 104	32.796 -29.333 29.418 -27.105	3.597 4.342	1.00	0.00	3A7
ATOM	501	Ö	ASN	104	29.471 -26.868	3.135	1.00	0.00	3A7
ATOM	502	N	ARG	105	28.961 -26.205	5.250	1.00	0.00	3A7
ATOM	503	CA	ARG	105	28.538 -24.859	4.929	1.00	0.00	3A7
ATOM	504	СВ	ARG	105	27.556 -24.275	5.967	1.00	0.00	3A7
ATOM	505	CG	ARG	105	26.214 -25.018	6.037	1.00	0.00	3A7
MOTA	506	CD	ARG	105	25.300 -24.418	7.111	1.00	0.00	3A7
ATOM	507	NE	ARG	105	24.029 -25.205	7.173	1.00	0.00	3A7 3A7
ATOM	508	CZ	ARG ARG	105	23.007 -24.845 21.860 -25.583	8.007 8.027		0.00 0.00	3A7 3A7
ATOM . ATOM	509 510		ARG	105 105	23.124 -23.752	8.816		0.00	3A7
ATOM	511	C	ARG	105	29.756 -23.977	4.884		0.00	3A7
ATOM	512	ō	ARG	105	30.703 -24.170	5.645		0.00	3A7
ATOM	513	N	ARG	106	29.750 -22.991	3.955	1.00	0.00	3A7
ATOM	514	CA	ARG	106	30.909 -22.177	3.639		0.00	3A7
ATOM	515	СВ	ARG	106	30.852 -21.586			0.00	3A7
ATOM	516	CG	ARG	106	30.675 -22.664	1.121		0.00	3A7
ATOM	517	CD	ARG	106	30.504 -22.088 31.739 -21.318	-0.292 -0.652		0.00	3A7 3A7
ATOM ATOM	518 519	NE CZ	ARG ARG	106 106	31.841 -20.619			0.00	3A7
ATOM	520		ARG	106	32.985 -19.927			0.00	3A7
ATOM	521		ARG	106	30.809 -20.607			0.00	3A7
ATOM	522	С	ARG		31.190 -21.087			0.00	3A7
ATOM	523	0	ARG	106	32.357 -20.971	5.015	1.00	0.00	3A7
MOTA	524	N	PRO		30.250 -20.287			0.00	3A7
ATOM	525	CA	PRO		30.565 -19.212			0.00	3A7
ATOM	526	CD	PRO		28.890 -20.159			0.00	3A7
ATOM	527	CB	PRO		29.245 -18.456			0.00	3A7 3A7
MOTA	528 529	CG	PRO PRO		28.480 -18.724 31.061 -19.732			0.00	3A7
MOTA MOTA	530	С 0	PRO		31.834 -19.045			0.00	3A7
MOTA	531	N	PHE		30.645 -20.949				3A7
ATOM	532	CA	PHE		30.989 -21.534				3A7

ATOM	533	СВ	PHE	108	29.984	-22.623	9.543	1.00	0.00	3A7
ATOM	534	CG	PHE	108	28.575		9.639	1.00	0.00	3A7
ATOM	535	CD1	PHE	108	27.823	-21.852	8.488	1.00	0.00	3A7
ATOM	536	CD2		108	27.969		10.885	1.00	0.00	3A7
ATOM	537	CE1		108	26.496		8.575	1.00	0.00	3A7
ATOM	538	CE2		108	26.638		10.976	1.00	0.00	3A7
ATOM	539	CZ	PHE	108	25.898		9.821	1.00	0.00	3A7
ATOM ATOM	540 541	С О	PHE PHE	108 108	32.360 33.016		9.070 10.095	1.00	0.00	3A7 3A7
ATOM	542	N	GLY	109	32.846		7.875	1.00	0.00	3A7
ATOM	543	CA	GLY	109	34.159		7.691	1.00	0.00	3A7
ATOM	544	c	GLY	109	35.333		8.056	1.00	0.00	3A7
ATOM	545	0	GLY	109	36.321		8.561	1.00	0.00	3A7
ATOM	546	N	PRO	110	35.267		7.853	1.00	0.00	3A7
ATOM	547	CA	PRO	110	36.311		8.270	1.00	0.00	3A7
MOTA	548	CD	PRO	110		-20.430	6.620	1.00	0.00	3A7
ATOM	549	СВ	PRO	110		-18.682	7.743	1.00	0.00	3A7
ATOM	550	CG	PRO	110	35.292		6.361	1.00	0.00	3A7
ATOM	551	C	PRO	110		-19.895	9.765	1.00	0.00	3A7
MOTA MOTA	552 553	N O	PRO VAL	110 111		-19.525 -20.153	10.094 10.690	1.00	0.00	3A7 3A7
MOTA	554	CA	VAL	111		-19.847	12.107	1.00	0.00	3A7
ATOM	555	СВ	VAL	111		-19.678	12.890	1.00	0.00	3A7
ATOM	556	CG1		111		-18.645	12.147	1.00	0.00	3A7
ATOM	557		VAL	111		-21.007	13.118	1.00	0.00	3A7
ATOM	558	С	VAL	111	36.707	-20.855	12.787	1.00	0.00	3A7
MOTA	559	0	VAL	111		-22.067	12.658	1.00	0.00	3A7
ATOM	560	N	GLY	112		-20.325	13.502	1.00	0.00	3A7
ATOM	561	CA	GLY	112		-21.102	14.130	1.00	0.00	3A7
ATOM	562	C	GLY	112		-20.384	13.863	1.00	0.00	3A7
ATOM ATOM	563 564	O N	GLY PHE	112 113		-19.155 -21.162	13.891 13.582	1.00	0.00	3A7 3A7
ATOM	565	CA	PHE	113		-20.640	13.182	1.00	0.00	3A7
ATOM	566	СВ	PHE	113		-20.476	14.380	1.00	0.00	3A7
ATOM	567	CG	PHE	113		-19.854	13.980	1.00	0.00	3A7
ATOM	568	CD1	PHE	113	45.891	-20.468	14.346	1.00	0.00	3A7
ATOM	569	CD2	PHE	113	44.738	-18.671	13.239	1.00	0.00	3A7
MOTA	570		PHE	113		-19.918	13.971	1.00	0.00	3A7
ATOM	571		PHE	113		-18.120	12.861	1.00	0.00	3A7
ATOM	572	CZ	PHE	113		-18.744	13.226	1.00	0.00	3A7
ATOM ATOM	573 574	C O	PHE PHE	113 113		-21.648 -22.372	12.181 12.431	1.00	0.00	3A7 3A7
ATOM	575	N	MET	114		-21.708	11.011	1.00	0.00	3A7
ATOM	576	CA	MET	114		-22.600	9.882	1.00	0.00	3A7
ATOM	577	СВ	MET	114		-22.624	9.331	1.00	0.00	3A7
ATOM	578	CG	MET	114	44.322	-21.313	8.647	1.00	0.00	3A7
ATOM	579	SD	MET	114		-19.936	9.761	1.00	0.00	3A7
ATOM	580	CE	MET	114		-18.779	8.440	1.00	0.00	3A7
ATOM	581	C	MET	114 .		-24.012	10.217	1.00	0.00	3A7
ATOM	582 583	O N	MET	114		-24.294 -24.924	11.346 9.208	1.00	0.00	3A7 3A7
ATOM ATOM	584	CA	LYS LYS	115 115		-26.343	9.268		0.00	3A7
ATOM	585	СВ	LYS	115		-27.158	10.423	1.00	0.00	3A7
ATOM	586	CG	LYS	115		-27.432	10.251	1.00	0.00	3A7
ATOM	587	CD	LYS	115		-26.252	10.533	1.00	0.00	3A7
ATOM	588	CE	LYS	115	44.796	-25.758	11.988	1.00	0.00	3A7
MOTA	589	NZ	LYS	115		-26.832	12.922	1.00	0.00	3A7
MOTA	590	C	LYS	115		-26.569	9.300	1.00	0.00	3A7
ATOM	591	0	LYS	115		-26.979	8.297	1.00	0.00	3A7
ATOM	592	N	ASN	116		-26.341	10.491	1.00	0.00	3A7
ATOM ATOM	593 594	CA CB	ASN ASN	116 116		-26.560 -25.724	10.889	1.00	0.00	3A7 3A7
ATOM	595	CG	ASN	116		-26.079	8.657	1.00	0.00	3A7
ATOM	596		ASN	116		-25.453	7.745	1.00	0.00	3A7
ATOM	597		ASN	116		-27.074	8.437	1.00	0.00	3A7
MOTA	598	С	ASN	116		-28.039	10.949	1.00	0.00	3A7
ATOM	599	0	ASN	116	38.029	-28.777	9.979	1.00	0.00	3A7
ATOM	600	N	ALA	117		-28.501	12.134	1.00	0.00	3A7
ATOM	601	CA	ALA	117		-29.900	12.415	1.00	0.00	3A7
ATOM	602	CB	ALA	117		-30.247	13.899	1.00	0.00	3A7
ATOM	603	C	ALA	117		-30.294	12.024	1.00	0.00	3A7
ATOM	604	0	ALA	117	33.542	-30.857	10.951	1.00	0.00	3A7

MOTA	605	N	ILE	118		-30.027	12.909	1.00	0.00	3A7
ATOM	606	CA	ILE	118		-30.498	12.732	1.00	0.00	3A7
ATOM	607	CB	ILE	118		-31.666 -32.948	13.661 13.008	1.00	0.00	3A7 3A7
ATOM ATOM	608 609	CG2 CG1	ILE	118 118		-31.523	15.000	1.00	0.00	3A7
ATOM	610	CD	ILE	118		-30.511	15.983	1.00	0.00	3A7
ATOM	611	С	ILE	118		-29.333	12.894	1.00	0.00	3A7
ATOM	612	0	ILE	118		-29.399	13.643	1.00	0.00	3A7
ATOM	613	N	SER	119		-28.231	12.139	1.00	0.00	3A7
ATOM ATOM	614 615	CA CB	SER SER	119 119		-27.054 -25.747	12.114 11.972	1.00	0.00 0.00	3A7 3A7
ATOM	616	OG	SER	119		-25.595	13.079	1.00	0.00	3A7
ATOM	617	C	SER	119		-27.178	10.949	1.00	0.00	3A7
ATOM	618	0	SER	119		-26.507	9.930	1.00	0.00	3A7
MOTA	619	N	ILE	120		-28.096	11.093	1.00	0.00	3A7
ATOM	620 621	CA CB	ILE	120 120		-28.576 -27.497	10.086 9.294	1.00	0.00	3A7 3A7
ATOM ATOM	622		ILE	120		-28.166	8.349	1.00	0.00	3A7
ATOM	623		ILE	120		-26.482	10.237	1.00	0.00	3A7
ATOM	624	CD	ILE	120	26.467	-27.096	11.166	1.00	0.00	3A7
MOTA	625	C	ILE	120		-29.507	9.171	1.00	0.00	3A7
ATOM	626	0	ILE	120		-29.081 -30.825	8.276 9.421	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	627 628	N CA	ALA ALA	121 121		-30.823	8.845	1.00	0.00	3A7
ATOM	629	CB	ALA	121		-32.322	9.891	1.00	0.00	3A7
ATOM	630	C	ALA	121		-32.895	8.190	1.00	0.00	3A7
MOTA	631	0	ALA	121		-33.051	8.369	1.00	0.00	3A7
ATOM	632	N	GLU	122		-33.699	7.384	1.00	0.00	3A7
ATOM ATOM	633 634	CA CB	GLU GLU	122 122		-34.785 -34.988	6.580 5.292	1.00	0.00	3A7 3A7
ATOM	635	CG	GLU	122		-33.676	4.532	1.00	0.00	3A7
ATOM	636	CD	GLU	122		-33.979	3.190	1.00	0.00	3A7
ATOM	637		GLU	122		-34.679	2.360	1.00	0.00	3A7
ATOM	638		GLU	122		-33.510	2.975	1.00	0.00	3A7
ATOM ATOM	639 640	С 0	GLU GLU	122 122		-36.057 -36.091	7.368 8.393	1.00	0.00 0.00	3A7 3A7
ATOM	641	N	ASP	123		-37.130	6.889	1.00	0.00	3A7
ATOM	642	CA	ASP	123		-38.402	7.576	1.00	0.00	3A7
ATOM	643	СВ	ASP	123		-39.195	7.107	1.00	0.00	3A7
ATOM	644	CG	ASP	123		-39.602	5.628	1.00	0.00	3A7
ATOM ATOM	645 646		ASP ASP	123 123		-38.707 -40.822	4.763 5.354	1.00	0.00	3A7 3A7
ATOM	647	C	ASP	123		-39.259	7.471	1.00	0.00	3A7
ATOM	648	0	ASP	123		-39.955	6.485	1.00	0.00	3A7
ATOM	649	N	GLU	124		-39.189	8.540	1.00	0.00	3A7
ATOM	650	CA	GLU	124		-39.870	8.683 7.609	1.00	0.00	3A7 3A7
ATOM ATOM	651 652	CB CG	GLU	124 124		-39.519 -40.257	7.793	1.00	0.00	3A7
ATOM	653	CD	GLU.	124		-39.851	6.672	1.00	0.00	3A7 .
ATOM	654	OE1	GLU	124		-39.275	6.989	1.00	0.00	3A7
MOTA	655		GLU	124		-40.115	5.486	1.00	0.00	3A7
ATOM	656	C	GLU	124		-39.381	10.020 10.866	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	657 658	O N	GLU	124 125		-40.149 -38.047	10.219	1.00	0.00	3A7
ATOM	659	CA	GLU	125		-37.358	11.455	1.00	0.00	3A7
ATOM	660	CB	GLU	125		-36.078	11.267	1.00	0.00	3A7
ATOM	661	CG	GLU	125		-36.303	10.505	1.00	0.00	3A7
ATOM	662	CD	GLU GLU	125 125		-37.314 -38.392	11.254 10.667	1.00	0.00	3A7 3A7
ATOM ATOM	663 664		GLU	125		-37.024	12.418	1.00	0.00	3A7
ATOM	665	C	GLU	125		-36.969	12.096	1.00	0.00	3A7
MOTA	666	0	GLU	125	31.785	~36.775	13.306	1.00	0.00	3A7
ATOM	667	N	TRP	126		-36.843	11.315	1.00	0.00	3A7
ATOM	668	CA	TRP	126		-36.458 -36.001	11.855 10.762	1.00	0.00	3A7 3A7
ATOM ATOM	669 670	CB CG	TRP TRP	126 126		-36.001	11.159	1.00		3A7 3A7
ATOM	671		TRP	126		-33.684	11.776	1.00		3A7
MOTA	672		TRP	126	26.092	-34.933	10.869	1.00		3A7
ATOM	673		TRP			-33.741	11.271	1.00		3A7
ATOM	674		TRP			-32.954 -33.139	11.818 12.252	1.00		3A7 3A7
ATOM ATOM	675 676		TRP TRP			-33.139 -31.670		1.00		3A7 3A7
	2.4	~~~				-				

ATOM	677	CZ3	TRP	126	28.868 -31.850	12.774	1.00	0.00	3A7
ATOM	678	CH2		126	27.680 -31.123	12.810	1.00	0.00	3A7
ATOM	679	c	TRP	126	28.874 -37.602	12.636	1.00	0.00	3A7
ATOM	680	ŏ	TRP	126	28.393 -37.423	13.750	1.00	0.00	3A7
ATOM	681	N	LYS	127	28.962 -38.842	12.090	1.00	0.00	3A7
				127	28.511 -40.060	12.743	1.00	0.00	3A7
ATOM	682	CA	LYS				1.00	0.00	3A7
ATOM	683	СВ	LYS	127	28.749 -41.279	11.833			3A7
ATOM	684	CG	LYS	127	28.086 -42.581	12.315	1.00	0.00	
ATOM	685	CD	LYS	127	28.264 -43.736	11.316	1.00	0.00	3A7
MOTA	686	CE	LYS	127	27.607 -45.046	11.770	1.00	0.00	3A7
ATOM	687	NZ	LYS	127	26.139 -44.893	11.883	1.00	0.00	3A7
ATOM	688	С	LYS	127	29.196 -40.320	14.072	1.00	0.00	3A7
ATOM	689	0	LYS	127	28.561 -40.651	15.070	1.00	0.00	3A7
MOTA	690	N	ARG	128	30.530 -40.112	14.123	1.00	0.00	3A7
ATOM	691	CA	ARG	128	31.301 -40.271	15.331	1.00	0.00	3A7
ATOM	692	СВ	ARG	128	32.812 -40.274	15.061	1.00	0.00	3A7
ATOM	693	CG	ARG	128	33.252 -41.515	14.267	1.00	0.00	3A7
ATOM	694	CD	ARG	128	34.765 -41.777	14.317	1.00	0.00	3A7
ATOM	695	NE	ARG	128	35.198 -41.942	15.749	1.00	0.00	3A7
ATOM	696	CZ	ARG	128	34.997 -43.090	16.469	1.00	0.00	3A7
ATOM	697		ARG	128	35.389 -43.140	17.776	1.00	0.00	3A7
ATOM	698		ARG	128	34.422 -44.186	15.894	1.00	0.00	3A7
					30.991 -39.217	16.367	1.00	0.00	3A7
MOTA	699	C	ARG	128					. 3A7
ATOM	700	0	ARG	128	30.847 -39.549	17.535	1.00	0.00	
ATOM	701	N	ILE	129	30.823 -37.931	15.976	1.00	0.00	3A7
ATOM	702	CA	ILE	129	30.486 -36.852	16.897	1.00	0.00	3A7
ATOM	703	СВ	ILE	129	30.651 -35.498	16.229	1.00	0.00	3A7
MOTA	704	CG2	ILE	129	29.684 -34.398	16.740	1.00	0.00	3A7
ATOM	705	CG1	ILE	129	32.104 -34.975	16.405	1.00	0.00	3A7
ATOM	706	CD	ILE	129	33.250 -35.944	16.093	1.00	0.00	3A7
ATOM	707	С	ILE	129	29.095 -37.028	17.444	1.00	0.00	3A7
ATOM	708	0	ILE	129	28.882 -36.896	18.640	1.00	0.00	3A7
ATOM	709	N	ARG	130	28.114 -37.398	16.595	1.00	0.00	3A7
ATOM	710	CA	ARG	130	26.759 ~37.661	17.021	1.00	0.00	3A7
ATOM	711	СВ	ARG	130	25.849 -37.943	15.811	1.00	0.00	3A7
ATOM	712	CG	ARG	130	25.540 -36.681	14.987	1.00	0.00	3A7
ATOM	713	CD	ARG	130	24.607 -36.942	13.796	1.00	0.00	3A7
ATOM	714	NE	ARG	130	25.280 -37.896	12.857	1.00	0.00	3A7
	715	CZ	ARG	130	24.691 -38.311	11.694	1.00	0.00	3A7
ATOM							1.00	0.00	3A7
ATOM	716		ARG	130	25.358 -39.169	10.868		0.00	3A7
ATOM	717		ARG	130	23.446 -37.869	11.351	1.00		3A7
ATOM	718	С	ARG	130	26.695 -38.843	17.970	1.00	0.00	
MOTA	719	0	ARG	130	26.037 -38.756	18.996	1.00	0.00	3A7
ATOM	720	N	SER	131	27.443 -39.943	17.701	1.00	0.00	3A7
MOTA	721	CA	SER	131	27.492 -41.105	18.571	1.00	0.00	3A7
ATOM	722	СВ	SER	131	28.322 -42.268	17.985	1.00	0.00	3A7
ATOM	723	OG	SER	131	29.697 -41.986		1.00	0.00	3A7
ATOM	724	С	SER	131	28.053 -40.816	19.936	1.00	0.00	3A7
ATOM	725	.0	SER	131	27.615 -41,352	20.947	1.00	0.00	. 3A7
ATOM	726	N	LEU	132	29.066 -39.936	19.998	1.00	0.00	3A7
ATOM	727	CA	LEU	132	29.705 -39.583	21.240	1.00	0.00	3A7
ATOM	728	СВ	LEU	132	31.017 -38.838	20.968	1.00	0.00	3A7
ATOM	729	CG	LEU	132	32.105 ~39.732	20.333	1.00	0.00	3A7
ATOM	730		LEU	132	33.135 -38.875			0.00	3A7
ATOM	731		LEU	132	32.782 -40.648			0.00	3A7
ATOM	732	c	LEU	132	28.808 -38.721			0.00	3A7
ATOM	733	ŏ	LEU	132	28.688 -38.937			0.00	3A7
ATOM	734	N	LEU	133	28.116 -37.745			0.00	3A7
	735	CA		133	27.269 -36.794			0.00	3A7
ATOM			LEU					0.00	3A7
ATOM	736	CB	LEU	133	26.997 -35.547				3A7
ATOM	737	CG	LEU	133	28.266 -34.787			0.00	3A7
MOTA	738		LEU	133	27.918 -33.493			0.00	
ATOM	739		LEU	133	29.211 -34.589			0.00	3A7
ATOM	740	С	LEU	133	25.928 -37.334			0.00	3A7
ATOM	741	0	LEU	133	25.403 -36.955			0.00	3A7
MOTA	742	N	SER		25.333 -38.237			0.00	3A7
MOTA	743	CA	SER		24.003 -38.748			0.00	3A7
ATOM	744	CB	SER	134	23.511 -39.662				3A7
MOTA	745	OG	SER	134	24.394 -40.706				3A7
MOTA	746	С	SER		23.800 -39.430	23.296	1.00	0.00	3A7
ATOM	747	0	SER		22.725 -39.220		1.00	0.00	3A7
ATOM	748	N	PRO		24.715 -40.198		1.00	0.00	3A7

ATOM	749	CA	PRO	135	24.491	-40.773	25.190	1.00	0.00	3A7
ATOM	750	CD	PRO	135		-40.834	23.260	1.00	0.00	3A7
ATOM	751	СВ	PRO	135	25.551	-41.871	25.355	1.00	0.00	3A7
MOTA	752	CG	PRO	135		-42.203	23.924	1.00	0.00	3A7
ATOM	753	C	PRO	135		-39.783	26.310	1.00	0.00	3A7
ATOM	754	0	PRO	135		-39.912	27.273	1.00	0.00	3A7
ATOM	755	N	THR	136		-38.805	26.231	1.00	0.00	3A7 3A7
ATOM	756	CA	THR	136 136) -37.840 3 -37.210	27.291 27.207	1.00	0.00	3A7
ATOM ATOM	757 758	CB OG1	THR THR	136		-37.210 5 -36.654	25.918	1.00	0.00	3A7
ATOM	759		THR	136		-38.319	27.492	1.00	0.00	3A7
ATOM	760	c	THR	136		3 -36.769	27.320	1.00	0.00	3A7
ATOM	761	0	THR	136		-36.212	28.360	1.00	0.00	3A7
ATOM	762	N	PHE	137	24.066	5 -36.471	26.165	1.00	0.00	3A7
ATOM	763	.CA	PHE	137		-35.454	26.069	1.00	0.00	3A7
ATOM	764	СВ	PHE	137		-34.665	24.778	1.00	0.00	3A7
ATOM	765	CG	PHE	137		33.645	25.018	1.00	0.00	3A7
ATOM	766		PHE	137		3 -33.792	24.468	1.00	0.00	3A7 3A7
ATOM	767 768		PHE PHE	137 137		7 -32.535 3 -32.863	25.831 24.725	1.00	0.00	3A7
ATOM ATOM	769		PHE	137		32.503	26.070	1.00	0.00	3A7
ATOM	770	CZ	PHE	137		6 -31.757	25.524	1.00	0.00	3A7
ATOM	771	c	PHE	137		1 -36.153	26.100	1.00	0.00	3A7
ATOM	772	0	PHE	137	20.77	9 -35.799	25.406	1.00	0.00	3A7
MOTA	773	N	THR	138	21.543	2 -37.179	26.952	1.00	0.00	3A7
ATOM	774	CA	THR	138		6 -37.782	27.179	1.00	0.00	3A7
MOTA	775	СВ	THR	138		3 -39.259	27.505	1.00	0.00	3A7
ATOM	776		THR	138		0 -39.549	28.518	1.00	0.00	3A7 3A7
ATOM	777		THR	138		340.035 8 -37.063	26.226 28.326	1.00	0.00	3A7
ATOM ATOM	778 779	С О	THR THR	138 138		4 -36.412	29.149	1.00	0.00	3A7
ATOM	780	N	SER	139		0 -37.211	28.416	1.00	0.00	3A7
ATOM	781	CA	SER	139		3 -36.585	29.427	1.00	0.00	3A7
ATOM	782	СВ	SER	139		7 -36.809	29.183	1.00	0.00	3A7
ATOM	783	OG	SER	139	15.59	0 -38.188	29.037	1.00	0.00	3A7
ATOM	784	С	SER	139 .		7 -37.053	30.810	1.00	0.00	3A7
MOTA	785	0	SER	139		8 -36.290	31.765	1.00	0.00	3A7
MOTA	786	N	GLY	140		3 -38.318	30.922	1.00	0.00	3A7
ATOM	787	CA	GLY	140		3 -38.898	32.158 32.618	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	788 789	C O	GLY GLY	140 140		2 -38.362 3 -38.260	33.820	1.00	0.00	3A7
ATOM	790	N	LYS	141		3 -38.021	31.673	1.00	0.00	3A7
ATOM	791	CA	LYS	141		9 -37.803	32.064	1.00	0.00	3A7
ATOM	792	СВ	LYS	141		5 -38.611	31.169	1.00	0.00	3A7
ATOM	793	CG	LYS	141	23.07	0 -40.129	31.293	1.00	0.00	3A7
MOTA	794	CD	LYS	141		0 -40.944	30.571	1.00	0.00	3A7
ATOM	795	CE	LYS	141		6 ~42.456	30.655	1.00	0.00	3A7
ATOM	796	NZ	LYS	141		8 -43.189 2 -36.386	29.928	1.00	0.00	3A7 3A7
ATOM ,	797 798	C O	LYS LYS	141 141	•	9 -35.680	32.232 33.265	1.00	0.Q0 0.00	3A7
ATOM	799	N	LEU	142		5 -36.031	31.185	1.00	0.00	3A7
ATOM	800	CA	LEU	142		4 -34.970	31.099	1.00	0.00	3A7
ATOM	801	СВ	LEU	142	23.97	2 -33.593	30.894	1.00	0.00	3A7
ATOM	802	CG	LEU	142	24.45	5 -32.799	29.656	1.00	0.00	3A7
ATOM	803		LEU	142		0 -31.564	29.439	1.00	0.00	3A7
ATOM	804		LEU	142		3 -32.407	29.718	1.00	0.00	3A7
ATOM	805	C	LEU	142		3 -34.903	32.241	1.00	0.00	3A7 3A7
ATOM	806	0	LEU	142		9 -33.901 9 -35.975	32.398 33.085	1.00	0.00	3A7
ATOM ATOM	807 808	N CA	LYS	143 143		1 -36.077	34.381	1.00	0.00	3A7
ATOM	809	СВ	LYS	143		35.966	34.315	1.00	0.00	3A7
ATOM	810	CG	LYS	143		7 -37.003	33.373		0.00	3A7
ATOM	811	CD	LYS	143		8 -38.480	33.614	1.00	0.00	3A7
ATOM	812	CE	LYS	143		4 -39.129		1.00	0.00	3A7
ATOM	813	NZ	LYS	143		7 -38.601	36.117		0.00	3A7
ATOM	814	C	LYS	143		31 -35.060		1.00	0.00	3A7
ATOM	815	0	LYS	143		51 -34.248	35.919		0.00	3A7 3A7
ATOM ATOM	816 817	N CA	GLU GLU	144 144		76 -35.097 93 -34.122			0.00	3A7
ATOM	818	CB	GLU	144		33 -34.122 38 -33.575			0.00	3A7
ATOM	819	CG	GLU	144		5 -34.669				3A7
ATOM	820	CD	GLU	144		30 -34.037				3A7

ATOM	821	OE1	GLU	144	25.849	-34.422	40.255	1.00	0.00	3A7
ATOM	822	OE2	GLU	144	24.022	-33.161	40.384	1.00	0.00	3A7
MOTA	823	С	GLU	144	23.380	-32.972	35.123	1.00	0.00	3A7
ATOM	824	0	GLU	144	24.284		34.907	1.00	0.00	3A7
ATOM	825	N	MET	145	22.163		34.523	1.00	0.00	3A7
ATOM	826		MET	145	21.768		33.757	1.00	0.00	3A7
ATOM	827	CB	MET	145	21.203		32.347	1.00	0.00	3A7 3A7
ATOM ATOM	828 829	CG SD	MET MET	145 145	20.243 19.496		32.238 30.593	1.00	0.00	3A7
ATOM	830	CE	MET	145	18.314		30.743	1.00	0.00	3A7
ATOM	831	C	MET	145	20.736		34.510	1.00	0.00	3A7
ATOM	832	ō	MET	145	20.810		34.599	1.00	0.00	3A7
ATOM	833	N	VAL	146	19.718		35.082	1.00	0.00	3A7
ATOM	834	CA	VAL .	146		-30.943	35.756	1.00	0.00	3A7
ATOM	835	CB	VAL	146	17.494	-31.869	36.146	1.00	0.00	3A7
MOTA	836	CG1		146		-30.982	36.556	1.00	0.00	3A7
ATOM	837	CG2		146		-32.759	34.935	1.00	0.00	3A7
MOTA	838	С	VAL	146		-30.148	36.957	1.00	0.00	3A7
ATOM	839	0	VAL	146		-29.004	37.094	1.00	0.00	3A7
ATOM	840	N	PRO	147		-30.644	37.801	1.00	0.00	3A7 3A7
ATOM ATOM	841 842	CA CD	PRO	147 147		-29.872 -32.060	38.908 37.960	1.00 1.00	0.00	3A7 3A7
ATOM	843	СВ	PRO PRO	147		-30.856	39.708	1.00	0.00	3A7
ATOM	844	CG	PRO	147		-32.213	39.420	1.00	0.00	3A7
ATOM	845	c	PRO	147		-28.672	38.470	1.00	0.00	3A7
ATOM	846	ō	PRO	147		-27.680	39.190	1.00	0.00	3A7
ATOM	847	N	ILE	148		-28.722	37.294	1.00	0.00	3A7
MOTA	848	CA	ILE	148	22.723	-27.631	36.762	1.00	0.00	3A7
ATOM	849	CB	ILE	148		-28.114	35.675	1.00	0.00	3A7
MOTA	850		ILE	148		-26.923	34.952	1.00	0.00	3A7
ATOM	851		ILE	148		-29.020	36.211	1.00	0.00	3A7
ATOM	852	CD	ILE	148		-30.116	37.225	1.00	0.00	3A7
MOTA	853	C	ILE	148		-26.558	36.204	1.00	0.00	3A7
ATOM	854	0	ILE	148		-25.361	36.322	1.00	0.00	3A7 3A7
ATOM ATOM	855 856	N CA	ILE	149 149		-26.968 -26.045	35.607	1.00	0.00	3A7
ATOM	857	CB	ILE	149		-26.744	34.263	1.00	0.00	3A7
ATOM	858		ILE	149		-25.733	33.743	1.00	0.00	3A7
ATOM	859		ILE	149		-27.390	33.058	1.00	0.00	3A7
ATOM	860	CD	ILE	149		-28.444	32.319	1.00	0.00	3A7
ATOM	861	С	ILE	149	19.032	-25.338	36.240	1.00	0.00	3A7
MOTA	862	0	ILE	149	18.779	-24.137	36.179	1.00	0.00	3A7
ATOM	863	N	ALA	150		-26.059	37.357	1.00	0.00	3A7
ATOM	864	CA	ALA	150		-25.493	38.558	1.00	0.00	3A7
ATOM	865	CB	ALA	150		-26.586	39.578	1.00	0.00	3A7 3A7
ATOM	866 867	C	ALA	150		-24.490 -23.461	39.195 39.693	1.00	0.00	3A7
ATOM ATOM	868	O N	ALA GLN	150 151		-24.737	39.144	1.00	0.00	3A7
ATOM	869	CA	GLN	151		-23.836	39.661	1.00	0.00	3A7
ATOM	870	СВ	GLN	151		-24.428	39.555	1.00	0.00	3A7
ATOM	871	CG	GLN	151		-25.483	40.637	1.00	0.00	3A7
ATOM	872	CD	GLN	151	24.551	-26.129	40.357	1.00	0.00	3A7
ATOM	873		GLN	151	25.580	-25.444	40.306	1.00	0.00	3A7
ATOM	874	NE2	GLN	151		-27.485	40.172	1.00	0.00	3A7
ATOM	875	C	GLN	151		-22.493	38.989	1.00	0.00	3A7
ATOM	876	0	GLN	151		-21.447	39.634	1.00	0.00	3A7
ATOM	877	N	TYR	152		-22.502	37.644	1.00	0.00	3A7
ATOM	878	CA	TYR	152		-21.288 -21.508	36.872 35.367	1.00	0.00	3A7 3A7
ATOM ATOM	879 880	CB CG	TYR TYR	152 152		-20.216	34.776	1.00	0.00	3A7
ATOM	881		TYR	152		-19.994	35.099	1.00	0.00	3A7
ATOM	882		TYR	152		-19.109	34.632	1.00	0.00	3A7
ATOM	883		TYR	152		-18.705	35.335	1.00	0.00	3A7
ATOM	884		TYR	152		-17.822	34.898	1.00	0.00	3A7
ATOM	885	CZ	TYR	152		-17.612	35.201	1.00	0.00	3A7
ATOM	886	ОН	TYR	152		-16.302	35.411	1.00	0.00	3A7
MOTA	887	С	TYR	152		-20.556	37.038	1.00	0.00	3A7
ATOM	888	0	TYR	152		-19.335	37.134	1.00	0.00	3A7
MOTA	889	N	GLY	153		-21.301	37.117	1.00	0.00	3A7
ATOM	890	CA	GLY	153		-20.733	37.311	1.00	0.00	3A7
ATOM	891	C	GLY	153		-19.972	38.591	1.00	0.00	3A7 3A7
ATOM	892	0	GLY	153	10.9//	-18.915	38.657	1.00	0.00	JAI

ATOM	893	N	ASP	154	18.270 -20	.457 3	39.650	1.00	0.00	3A7
ATOM	894	CA	ASP	154	18.353 -19		0.919	1.00	0.00	3A7
ATOM	895	СВ	ASP	154	19.017 -20		1.976		0.00	3A7
									0.00	3A7
ATOM	896	CG	ASP	154	18.142 -21		12.299			
ATOM	897	OD1		154	16.975 -21		11.830		0.00	3A7
MOTA	898	OD2	ASP	154	18.643 -22	.790 4	13.039	1.00	0.00	3A7
ATOM	899	С	ASP	154	19.130 -18	.483 4	10.808	1.00	0.00	3A7
ATOM	900	0	ASP	154	18.726 -17	.469 4	11.361	1.00	0.00	3A7
	901	N	VAL	155	20.243 -18		10.041	1.00	0.00	3A7
ATOM										
ATOM	902	CA	VAL	155	21.039 -17		39.761	1.00	0.00	3A7
ATOM	903	CB	VAL	155	22.308 -17	.637	38.989	1.00	0.00	3A7
ATOM	904	CG1	VAL	155	23.103 -16	.370	38.590	1.00	0.00	3A7
ATOM	905	CG2	VAL	155	23.251 -18	.537	39.870	1.00	0.00	3A7
ATOM	906	C	VAL	155	20.273 -16		39.005	1.00	0.00	3A7
					20.407 -15		39.286	1.00	0.00	3A7
ATOM	907	0	VAL	155						
ATOM	908	N	LEU	156	19.427 -16		38.035	1.00	0.00	3A7
ATOM	909	CA	LEU	156	18.566 -15	.759	37.295	1.00	0.00	3A7
ATOM	910	СВ	LEU	156	17.791 -16	.496	36.208	1.00	0.00	3A7
ATOM	911	CG	LEU	156	17.040 -15	.502	35.295	1.00	0.00	3A7
ATOM	912		LEU	156	17.539 -15		33.841	1.00	0.00	3A7
										3A7
ATOM	913		LEU	156	15.520 -15		35.345	1.00	0.00	
ATOM	914	С	LEU	156	17.570 -15		38.134	1.00	0.00	3A7
ATOM	915	0	LEU	156	17.442 -13	.817	38.081	1.00	0.00	3A7
MOTA	916	N	VAL	157	16.840 -15	.805	38.969	1.00	0.00	3A7
ATOM	917	CA	VAL	157	15.830 -15		39.861	1.00	0.00	3A7
ATOM			VAL	157	15.164 -16		40.629	1.00	0.00	3A7
	918	СВ								
ATOM	919		VAL	157	14.204 -15		41.728	1.00	0.00	3A7
ATOM	920	CG2	VAL	157	14.373 -17		39.609	1.00	0.00	3A7
ATOM	921	С	VAL	157	16.437 -14	.314	40.832	1.00	0.00	3A7
ATOM	922	0	VAL	157	15.906 -13	.236	41.069	1.00	0.00	3A7
ATOM	923	N	ARG	158	17.626 -14		41.358	1.00	0.00	3A7
ATOM	924	CA	ARG	158	18.365 -13		42.251	1.00	0.00	3A7
										3A7
ATOM	925	CB	ARG	158	19.590 -14		42.789	1.00	0.00	
ATOM	926	CG	ARG	158	20.308 -13		43.961	1.00	0.00	3A7
ATOM	927	CD	ARG	158	21.475 -14	1.689	44.519	1.00	0.00	3A7
MOTA	928	NE	ARG	158	20.932 -19	.988	45.038	1.00	0.00	3A7
ATOM	929	CZ	ARG	158	21.742 -1	.042	45.358	1.00	0.00	3A7
ATOM	930		ARG	158	21.187 -18		45.808	1.00	0.00	3A7
	931		ARG	158	23.097 -10		45.230	1.00	0.00	3A7
ATOM										3A7
ATOM	932	С	ARG	158	18.810 -13		41.638	1.00	0.00	
ATOM	933	О	ARG	158	18.732 -1		42.274	1.00	0.00	3A7
ATOM	934	N	ASN	159	19.237 -1 3	2.550	40.359	1.00	0.00	3A7
ATOM	935	CA	ASN	159	19.621 -1	1.357	39.637	1.00	0.00	3A7
ATOM	936	CB	ASN	159	20.171 -1	1.697	38.250	1.00	0.00	3A7
ATOM	937	CG	ASN	159	21.490 -1		38.358	1.00	0.00	3A7
ATOM	938		ASN	159	22.072 -1		39.439	1.00	0.00	3A7
										3A7
ATOM	939		ASN	159	21.964 -1		37.177	1.00	0.00	
ATOM	940	С	ASN	159	18.466 -1		39.454	1.00	0.00	3A7
ATOM	941	0	ASN.	159	18.606 -	9.195	39.568	1.00	0.00	3A7
ATOM	942	N	LEU	160	17.267 -1	0.966	39.205	1.00	0.00	3A7
ATOM	943	CA	LEU	160	16.066 -1	0.198	39.031	1.00	0.00	3A7
ATOM	944	СВ	LEU	160	14.972 -1		38.383	1.00	0.00	3A7
					15.234 -1		36.902	1.00	0.00	3A7
MOTA	945	CG	LEU	160						
ATOM	946		LEU	160	14.149 -1		36.402	1.00	0.00	3A7
ATOM	947	CD2	LEU	160	15.359 -1	0.246	35.959	1.00	0.00	3A7
ATOM	948	С	LEU	160	15.557 -	9.655	40.349	1.00	0.00	3A7
ATOM	949	0	LEU	160	14.965 -	8.580	40.420	1.00	0.00	3A7
ATOM	950	N	ARG	161	15.836 -1		41.455	1.00	0.00	3A7
ATOM	951	CA	ARG	161		9.958	42.787	1.00	0.00	3A7
										3A7
ATOM	952	CB	ARG	161	15.773 -1		43.830	1.00	0.00	
ATOM	953	CG	ARG	161	14.640 -1	2.097	43.887	1.00	0.00	3A7
MOTA	954	CD	ARG	161	14.752 -1	3.097	45.047	1.00	0.00	3A7
MOTA	955	NE	ARG	161	15.964 -1	3.954	44.841	1.00	0.00	3A7
ATOM	956	CZ	ARG	161	16.221 -1		45.617	1.00	0.00	3A7
ATOM	957		ARG	161	17.333 -1		45.374	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	958		ARG	161	15.375 -1		46.629			
MOTA	959	C	ARG	161		8.712	43.210	1.00	0.00	3A7
ATOM	960	0	ARG	161		7.843	43.879	1.00	0.00	3A7
ATOM	961	N	ARG	162	17.510 -	8.597	42.792	1.00	0.00	3A7
ATOM	962	CA	ARG	162		7.499	43.134	1.00	0.00	3A7
ATOM	963	СВ	ARG	162		7.869	42.894	1.00		3A7
	964	CG	ARG	162		8.986	43.829	1.00		3A7
MOTA	204	CG	ANG	104	20.340	0.500	33.023	1.00	5.00	J

ATOM	965	CD	ARG	162	21.838	-9.302	43.666	1.00	0.00	3A7
ATOM	966	NE	ARG	162	22.095	-9.696	42.242	1.00	0.00	3A7
MOTA	967	CZ	ARG	162	23.363	-9.855	41.755	1.00	0.00	3A7
MOTA	968	NH1		162	23.548 -		40.433	1.00	0.00	3A7
MOTA	969	NH2		162	24.444	-9.724	42.577	1.00	0.00	3A7
MOTA	970	C	ARG	162	18.080	-6.236	42.355	1.00	0.00	3A7 3A7
MOTA	971	0	ARG	162	18.755	-5.220	42.500 41.519	1.00	0.00	3A7
ATOM ATOM	972 973	N CA	GLU GLU	163 163	17.014 16.615	-6.247 -5.103	40.744	1.00	0.00	3A7
ATOM	974	CB	GLU	163	15.965	-5.504	39.413	1.00	0.00	3A7
ATOM	975	CG	GLU	163	16.981	-6.330	38.605	1.00	0.00	3A7
ATOM	976	CD	GLU	163	16.426	-6.716	37.246	1.00	0.00	3A7
ATOM	977	OE1		163	17.080	-6.372	36.227	1.00	0.00	3A7
ATOM	978		GLU	163	15.354	-7.376	37.210	1.00	0.00	3A7
ATOM	979	С	GLU	163	15.784	-4.183	41.582	1.00	0.00	3A7
ATOM	980	0	GLU	163	15.662	-2.998	41.288	1.00	0.00	3A7
MOTA	981	N	ALA	164	15.230	-4.708	42.699	1.00	0.00	3A7
MOTA	982	CA	ALA	164	14.728	-3.939	43.812	1.00	0.00	3A7
ATOM	983	CB	ALA	164	15.779	-2.963	44.394	1.00	0.00	3A7
ATOM	984	C	ALA	164	13.480	-3.200 -1.993	43.529 43.644	1.00 1.00	0.00	3A7 3A7
MOTA MOTA	985 986	O N	ALA GLU	164 165	13.505 12.363	-3.878	43.176	1.00	0.00	3A7
ATOM	987	CA	GLU	165	10.993	-3.400	43.222	1.00	0.00	3A7
ATOM	988	CB	GLU	165	10.561	-2.688	44.540	1.00	0.00	3A7
ATOM	989	CG	GLU	165	10.851	-3.510	45.809	1.00	0.00	3A7
ATOM	990	CD	GLU	165	10.308	-2.803	47.050	1.00	0.00	3A7
ATOM	991	OE1	GLU	165	9.757	-1.678	46.915	1.00	0.00	3A7
ATOM	992	OE2	GLU	165	10.441	-3.390	48.158	1.00	0.00	3A7
ATOM	993	С	GLU	165	10.541	-2.574	42.031	1.00	0.00	3A7
MOTA	994	0	GLU	165	9.403	-2.728	41.595	1.00	0.00	3A7
MOTA	995	N	THR	166	11.382	-1.661	41.488	1.00	0.00	3A7
ATOM	996	CA	THR	166	10.979	-0.758	40.425	1.00	0.00	3A7
ATOM	997	CB	THR	166	10.351	0.509	40.932	1.00	0.00	3A7 3A7
ATOM	998		THR	166	9.175	0.217 1.442	41.676 39.767	1.00	0.00 0.00	3A7
ATOM ATOM	999 1000	C	THR THR	166 166	9.944 12.235	-0.374	39.728	1.00	0.00	3A7
ATOM	1000	Ö	THR	166	12.410	-0.652	38.547	1.00	0.00	3A7
ATOM	1002	N	GLY	167	13.141	0.230	40.560	1.00	0.00	3A7
ATOM	1003	CA	GLY	167	14.556	0.524	40.415	1.00	0.00	3A7
ATOM	1004	С	GLY	167	14.980	0.965	39.058	1.00	0.00	3A7
MOTA	1005	0	GLY	167	15.037	2.155	38.750	1.00	0.00	3A7
MOTA	1006	N	LYS	168	15.246	-0.048	38.208	1.00	0.00	3A7
MOTA	1007	CA	LYS	168	15.423	0.121	36.801	1.00	0.00	3A7
MOTA	1008	СВ	LYS	168	16.887	-0.172	36.380	1.00	0.00	3A7
ATOM	1009	CG	LYS	168	17.309	0.475	35.050	1.00	0.00	3A7 3A7
ATOM ATOM	1010 1011	CD CE	LYS	168 168	18.803 19.236	0.294 -1.160	34.725 34.483	1.00	0.00	3A7
ATOM	1011	NZ	LYS LYS	168	18.558	-1.731	33.297	1.00	0.00	3A7
ATOM	1013	C	LYS	168	14.438	-0.857	36.181	1.00	0.00	3A7
ATOM	1014	õ	LYS	168	14.315	-1.969	36.694	1.00	0.00	3A7
MOTA	1015	N	PRO	169	13.751	-0.544	35.061	1.00	0.00	3A7
MOTA	1016	CA	PRO	169	13.228	-1.488	34.077	1.00	0.00	3A7
MOTA	1017	CD	PRO	169	13.706	0.834	34.565	1.00	0.00	3 A 7
ATOM	1018	CB	PRO	169	12.639	-0.568	33.005	1.00	0.00	3A7
MOTA	1019	CG	PRO	169	13.438	0.725	33.072	1.00	0.00	3A7
ATOM	1020	C	PRO	169	14.386	-2.289	33.508	1.00	0.00	3A7
ATOM	1021	0	PRO	169	15.533	-1.866	33.608	1.00	0.00	3A7 3A7
ATOM	1022	N	VAL	170	14.110	-3.480	32.963 32.688	1.00	0.00	3A7 3A7
MOTA MOTA	1023 1024	CA CB	VAL VAL	170 170	15.120 14.791	-4.462 -5.773	33.379		0.00	3A7
ATOM	1024		VAL	170	15.992	-6.742	33.323	1.00	0.00	3A7
ATOM	1026		VAL	170	14.350	-5.485	34.825	1.00	0.00	3A7
ATOM	1027	¢	VAL	170	15.190	-4.659	31.200		0.00	3A7
ATOM	1028	ŏ	VAL	170	14.185	-4.556	30.501	1.00	0.00	3A7
ATOM	1029	N	THR	171	16.400	-4.984	30.690		0.00	3A7
MOTA	1030	CA	THR	171	16.616	-5.364	29.321	1.00	0.00	3A7
MOTA	1031	СВ	THR	171	17.889	-4.784	28.730		0.00	3A7
MOTA	1032	0G1		171	17.858	-3.368			0.00	3A7
ATOM	1033	CG2		171	18.018	-5.145			0.00	3A7
ATOM	1034	С	THR	171	16.717	-6.854	29.319		0.00	3A7
ATOM	1035	0	THR	171	17.667	-7.434				3A7 3A7
MOTA	1036	N	LEU	172	15.716	-7.527	28.719	1.00	0.00	241

ATOM	1037	CA	LEU	172	15.566	-8.955	28.820	1.00	0.00	3A7
ATOM	1038	СВ	LEU	172	14.147	-9.409	28.421	1.00	0.00	3A7
	1039	CG		172	12.958	-8.735	29.139	1.00	0.00	3A7
ATOM			LEU						0.00	3A7
MOTA	1040	CD1		172	13.118	-8.664	30.670	1.00		
ATOM	1041	CD2		172	12.633	-7.378	28.501	1.00	0.00	3A7
ATOM	1042	С	LEU	172	16.574	-9.705	27.991	1.00	0.00	3A7
MOTA	1043	0	LEU	172	17.033 -	-10.771	28.384	1.00	0.00	3A7
ATOM	1044	N	LYS	173	16.994	-9.161	26.826	1.00	0.00	3A7
ATOM	1045	CA	LYS	173	17.961	-9.803	25.952	1.00	0.00	3A7
					18.202	-8.967	24.685	1.00	0.00	3A7
ATOM	1046	CB	LYS	173					0.00	3A7
ATOM	1047	CG	LYS	173	19.033	-9.687	23.605	1.00		
MOTA	1048	CD	LYS	173	19.257	-8.825	22.357	1.00	0.00	3A7
MOTA	1049	CE	LYS	173	19.931	-9.589	21.211	1.00	0.00	3A7
ATOM	1050	NZ	LYS	173	20.065	-8.725	20.017	1.00	0.00	3A7
ATOM	1051	С	LYS	173	19.296	-10.057	26.620	1.00	0.00	3A7
ATOM	1052	0	LYS	173	19.912	-11.106	26.445	1.00	0.00	3A7
ATOM	1053	N	HIS	174	19.729	-9.103	27.472	1.00	0.00	3A7
							28.204	1.00	0.00	3A7
MOTA	1054	CA	HIS	174	20.962	-9.190				
MOTA	1055	ND1		174	23.840	-7.893	28.844	1.00	0.00	3A7
ATOM	1056	CG	HIS	174	22.644	-7.783	29.521	1.00	0.00	3A7
ATOM	1057	CB	HIS	174	21.288	-7.846	28.865	1.00	0.00	3A7
MOTA	1058	NE2	HIS	174	24.347	-7.664	30.996	1.00	0.00	3A7
ATOM	1059	CD2		174	22.973	-7.645	30.834	1.00	0.00	3A7
ATOM	1060		HIS	174	24.824	-7.814	29.775	1.00	0.00	3A7
					20.970		29.275	1.00	0.00	3A7
MOTA	1061	С	HIS	174						
ATOM	1062	0	HIS	174	21.877		29.317	1.00	0.00	3A7
MOTA	1063	N	VAL	175	19.954		30.170	1.00	0.00	3A7
ATOM	1064	CA	VAL	175	19.876	-11.181	31.303	1.00	0.00	3A7
MOTA	1065	CB	VAL	175	18.832	-10.715	32.291	1.00	0.00	3A7
MOTA	1066	CG1	VAL	175	18.836	-11.586	33.568	1.00	0.00	3A7
ATOM	1067		VAL	175	19.117	-9.239	32.645	1.00	0.00	3A7
ATOM	1068	C	VAL	175	19.575		30.872	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	1069	0	VAL	175	20.055		31.455			
ATOM	1070	N	PHE	176	18.769		29.799	1.00	0.00	3A7
ATOM	1071	CA	PHE	176	18.383		29.302	1.00	0.00	3A7
MOTA	1072	CB	PHE	176	17.044	-13.978	28.573	1.00	0.00	3A7
MOTA	1073	CG	PHE	176	15.984	-14.019	29.651	1.00	0.00	3A7
ATOM	1074	CD1	PHE	176	15.271	-12.887	30.048	1.00	0.00	3A7
ATOM	1075		PHE	176	15.760		30.337	1.00	0.00	3A7
ATOM	1076		PHE	176		-12.941	31.117	1.00	0.00	3A7
						-15.282	31.394	1.00	0.00	3A7
ATOM	1077		PHE	176						3A7
ATOM	1078	CZ	PHE	176		-14.139	31.790	1.00	0.00	
MOTA	1079	С	PHE	176		-14.648	28.382	1.00	0.00	3A7
ATOM	1080	0	PHE	176	19.429	-15.860	28.180	1.00	0.00	3A7
ATOM	1081	N	GLY	177	20.328	-13.824	27.829	1.00	0.00	3A7
ATOM	1082	CA	GLY	177	21.447	-14.314	27.061	1.00	0.00	3A7
ATOM	1083	С	GLY	177	22,530	-14.791	27.997	1.00	0.00	3A7
ATOM	1084	ō	GLY	177		-15.756	27.714	1.00	0.00	3A7
ATOM	1085	N	ALA	178		-14.142	29.180	1.00	0.00	3A7
	-				•		30.214	1.00	0.00	3A7
MOTA	1086	CA	ALA	178		-14.483				3A7
MOTA	1087	СВ	ALA	178		-13.426	31.327	1.00	0.00	
MOTA	1088	С	ALA	178		-15.805	30.855	1.00	0.00	3A7
ATOM	1089	0	ALA	178	24.178	-16.635	31.070	1.00	0.00	3A7
ATOM	1090	N	TYR	179	22.004	-16.063	31.127	1.00	0.00	3A7
ATOM	1091	CA	TYR	179	21.522	-17.288	31.732	1.00	0.00	3A7
ATOM	1092	СВ	TYR	179		-17.174	31.929	1.00	0.00	3A7
ATOM	1093	CG	TYR	179		-18.432	31.952	1.00	0.00	3A7
			TYR			-18.892	33.140	1.00	0.00	3A7
ATOM	1094			179						3A7
MOTA	1095		TYR	179		-19.133	30.778	1.00	0.00	
ATOM	1096	CEI	TYR	179		-20.112	33.200		0.00	3A7
MOTA	1097	CE2	TYR	179		-20.354	30.824		0.00	3A7
MOTA	1098	CZ	TYR	179	17.709	-20.868	32.046	1.00	0.00	3A7
MOTA	1099	OH	TYR	179	17.108	-22.143	32.117	1.00	0.00	3A7
ATOM	1100	Ċ	TYR	179		-18.504	30.914			3A7
ATOM	1101	ŏ	TYR	179		-19.487	31.413			3A7
										3A7
ATOM	1102	N	SER			-18.432				
MOTA	1103	CA	SER	180		-19.553				3A7
MOTA	1104	СВ	SER			-19.328				3A7
MOTA	1105	OG	SER	180	21.331	-18.109	26.860	1.00		3A7
MOTA	1106	С	SER		23.198	-19.852	28.402	1.00	0.00	3A7
ATOM	1107	0	SER			-21.010		1.00	0.00	3A7
ATOM	1108	N	MET			-18.834				3A7
A. O.1	1100	.,		101	24.004	20.007				2.47

ATOM	1109	CA	MET	181	25.507 -				0.00	3A7
ATOM	1110	CB	MET	181	26.246 -				0.00	3A7
MOTA	1111	CG	MET	181	25.986			1.00	0.00	3A7 3A7
MOTA	1112	SD	MET	181	26.894 - 25.919 -		26.130 27.203	1.00	0.00 0.00	3A7
ATOM ATOM	1113 1114	CE	MET MET	181 181	26.127		29.282	1.00	0.00	3A7
ATOM ATOM	1115	0	MET	181	26.923		29.117	1.00	0.00	3A7
ATOM	1116	N	ASP	182	25.695		30.493	1.00	0.00	3A7
ATOM	1117	CA	ASP	182	26.174		31.695	1.00	0.00	3A7
ATOM	1118	СВ	ASP	182	25.809	-19.160	32.908	1.00	0.00	3A7
ATOM	1119	CG	ASP	182	26.545		32.877	1.00	0.00	3A7
MOTA	1120		ASP	182	27.380		31.961	1.00	0.00	3A7
MOTA	1121		ASP	182	26.276		33.788	1.00	0.00	3A7 3A7
ATOM	1122	C	ASP	182	25.645 26.371		31.886 32.382	1.00	0.00	3A7
ATOM ATOM	1123 1124	O N	ASP Val	182 183	24.401		31.448	1.00	0.00	3A7
ATOM	1125	CA	VAL	183	23.887		31.514	1.00	0.00	3A7
ATOM	1126	СВ	VAL	183	22.419		31.124	1.00	0.00	3A7
ATOM	1127		VAL	183	21.919		30.984	1.00	0.00	3A7
MOTA	1128	CG2	VAL	183	21.578	-22.468	32.200	1.00	0.00	3A7
ATOM	1129	С	VAL	183	24.678		30.610	1.00	0.00	3A7
MOTA	1130	0	VAL	183	25.065		31.027	1.00	0.00	3A7
ATOM	1131	N	ILE	184	24.999		29.353	1.00	0.00	3A7 3A7
ATOM	1132	CA	ILE	184	25.762 25.800		28.439 27.039	1.00	0.00	3A7
ATOM	1133	CB	ILE ILE	184 184	26.594		26.093	1.00	0.00	3A7
ATOM ATOM	1134 1135		ILE	184	24.365		26.489	1.00	0.00	3A7
ATOM	1136	CD	ILE	184	23.531		26.404	1.00	0.00	3A7
ATOM	1137	c	ILE	184	27.167		28.928	1.00	0.00	3A7
ATOM	1138	0	ILE	184	27.720	-25.652	28.859	1.00	0.00	3A7
MOTA	1139	N	THR	185		-23.489	29.486	1.00	0.00	3A7
ATOM	1140	CA	THR	185		-23.511	30.002	1.00	0.00	3A7
MOTA	1141	CB	THR	185		-22.111	30.359	1.00	0.00 0.00	3A7 3A7
ATOM	1142		THR	185 185		-21.307 -22.108	29.187 30.943	1.00	0.00	3A7
ATOM ATOM	1143 1144	CG2	THR THR	185		-24.418	31.192	1.00	0.00	3A7
ATOM	1145	ŏ	THR	185		-25.166	31.343	1.00	0.00	3A7
ATOM	1146	N	SER	186		-24.404	32.066	1.00	0.00	3A7
MOTA	1147	CA	SER	186	28.262	-25.188	33.262	1.00	0.00	3A7
MOTA	1148	СВ	SER	186		-24.719	34.259	1.00	0.00	3A7
ATOM	1149	OG	SER	186		-23.412	34.719	1.00	0.00	3A7 3A7
MOTA	1150	C	SER	186		-26.655	33.000 33.598	1.00	0.00 0.00	3A7
ATOM ATOM	1151 1152	O N	SER THR	186 187		-27.500 -27.006	32.060	1.00	0.00	3A7
ATOM	1153	CA	THR	187		-28.386	31.711	1.00	0.00	3A7
ATOM	1154	СВ	THR	187		-28.580	30.943	1.00	0.00	3A7
ATOM	1155		THR	187		-27.748	29.789	1.00	0.00	3A7
ATOM	1156	CG2	THR	187		-28.285	31.861	1.00	0.00	3A7
MOTA	1157	С	THR	187 ,		-28.983	30.897	1,00	0.00	3A7
ATOM	1158	0	THR	187		-30.195	30.899	1.00	0.00	3A7 3A7
ATOM	1159 1160	N CA	SER	188 188		-28.115 -28.556	30.176 29.280	1.00		3A7
ATOM ATOM	1160	CB	SER SER	188		-27.697	27.991	1.00	0.00	3A7
ATOM	1162		SER	188		-26.347	28.250	1.00	0.00	3A7
ATOM	1163		SER	188		-28.690	29.970	1.00	0.00	3A7
MOTA	1164		SER	188	31.803	-29.681	29.768	1.00	0.00	3A7
MOTA	1165	N	PHE	189		-27.672	30.766			3A7
MOTA	1166		PHE	189		-27.581	31.256			3A7
MOTA	1167		PHE	189		-26.363	30.732			3A7 3A7
ATOM	1168		PHE	189		-26.027 -24.694	29.300 28.976			3A7
ATOM ATOM	1169 1170		PHE PHE	189 189		-26.986				3A7
ATOM	1170		l PHE	189		-24.317				3A7
ATOM	1172		2 PHE	189		-26.618				3A7
ATOM	1173		PHE	189	32.933	-25.284	26.668	1.00		3A7
ATOM	1174	С	PHE	189		-27.463				3A7
MOTA	1175		PHE	189		-27.441				3A7
ATOM	1176		GLY	190		-27.378				3A7 3A7
ATOM	1177		GLY	190		-27.345 -25.956				3A7
ATOM ATOM	1178 1179		GLY GLY	190 190		-25.095				3A7
ATOM	1180		VAL	191		-25.744				3A7

ATOM	1181	CA	VAL	191	33.597 -2	4.510	36.596	1.00	0.00	3A7
ATOM	1182		VAL	191	33.426 -2	3.250	35.727	1.00	0.00	3A7
ATOM	1183	CG1	VAL	191	32.199 -2	2.372	36.078	1.00	0.00	3A7
ATOM	1184	CG2	VAL	191	34.729 -2		35.812	1.00	0.00	3A7
ATOM	1185	С	VAL	191	33.100 -2		38.012	1.00	0.00	3A7
MOTA	1186	0	VAL	191	31.935 -2	4.551	38.325	1.00	0.00	3A7
MOTA	1187	N	SER	192	34.012 -2		38.900	1.00	0.00	3A7
ATOM	1188	CA	SER	192	33.727 -2		40.281	1.00	0.00	3A7
ATOM	1189	СВ	SER	192	34.779 -2		41.252	1.00	0.00	3A7
ATOM	1190	OG	SER	192	34.799 -2		41.156	1.00	0.00	3A7
ATOM	1191	C	SER	192	33.716 -2		40.410	1.00	0.00	3A7
MOTA	1192	0	SER	192	34.136 -2		39.501	1.00	0.00	3A7 3A7
ATOM	1193	N	ILE	193	33.230 -2 33.138 -2		41.572 41.867	1.00	0.00	3A7 3A7
ATOM	1194	CA CB	ILE	193 193	31.890 -1		42.671	1.00	0.00	3A7
ATOM ATOM	1195 1196	CG2		193	31.794 -1		42.861	1.00	0.00	3A7
ATOM	1197	CG1		193	30.615 -2		41.992	1.00	0.00	3A7
ATOM	1198	CD	ILE	193	30.351 -1		40.581	1.00	0.00	3A7
ATOM	1199	c	ILE	193	34.389 -1		42.618	1.00	0.00	3A7
ATOM	1200	ō	ILE	193	34.518 -1		43.816	1.00	0.00	3A7
ATOM	1201	N	ASP	194	35.344 -1		41.887	1.00	0.00	3A7
ATOM	1202	CA	ASP	194	36.617 -1	8.685	42.420	1.00	0.00	3A7
ATOM	1203	СВ	ASP	194	37.706 -1	9.786	42.267	1.00	0.00	3A7
ATOM	1204	CG	ASP	194	38.984 -1	9.433	43.034	1.00	0.00	3A7
ATOM	1205	OD1	ASP	194	38.899 -1	9.270	44.280	1.00	0.00	3A7
ATOM	1206	OD2	ASP	194	40.056 -1	9.326	42.381	1.00	0.00	3A7
MOTA	1207	С	ASP	194	36.993 -1		41.654	1.00	0.00	3A7
MOTA	1208	0	ASP	194	37.756 -1		42.141	1.00	0.00	3A7
ATOM	1209	N	SER	195	36.443 -1		40.420	1.00	0.00	3A7
ATOM	1210	CA	SER	195	36.648 -1		39.548	1.00	0.00	3A7
MOTA	1211	CB	SER	195	36.679 -1		38.055	1.00	0.00	3A7 3A7
MOTA	1212	OG	SER	195	37.748 -1 35.523 -1		37.811 39.763	1.00	0.00 0.00	3A7
ATOM	1213	C	SER	195	34.456 -1		40.256	1.00	0.00	3A7
MOTA MOTA	1214 1215	O N	SER LEU	195 196	35.759 -1		39.386	1.00	0.00	3A7
ATOM	1215	CA	LEU	196	34.826 -1		39.580	1.00	0.00	3A7
ATOM	1217	СВ	LEU	196	35.494 -1		40.138	1.00	0.00	3A7
ATOM	1218	CG	LEU	196	36.127 -1		41.551	1.00	0.00	3A7
ATOM	1219		LEU	196	35.140 -1		42.599	1.00	0.00	3A7
ATOM	1220		LEU	196	37.469 -1	12.399	41.574	1.00	0.00	3A7
ATOM	1221	С	LEU	196	34.175 -1	12.481	38.258	1.00	0.00	3A7
ATOM	1222	0	LEU	196	33.796 -	11.334	38.022	1.00	0.00	3A7
ATOM	1223	N	ASN	197	34.036 -		37.366	1.00	0.00	3A7
MOTA	1224	CA	ASN	197	33.382 -		36.068	1.00	0.00	3A7
ATOM	1225	СВ	ASN	197	31.946 -		36.138	1.00	0.00	3A7
ATOM	1226	CG	ASN	197	31.125 -		34.865	1.00	0.00	3A7 3A7
ATOM	1227		ASN	197	31.170 -:		34.295 34.431	1.00	0.00	3A7
ATOM ATOM	1228 1229	C ND2	ASN ASN	197 197	30.353 -: 34.255 -:		35.072	1.00	0.00	3A7
ATOM	1230	Ö	ASN	197	33.812 -		34.419	1.00	0.00	3A7
ATOM	1231	N	ASN	198	35.541 -		34.960	1.00	0.00	3A7
ATOM	1232	CA	ASN	198	36.520 -			1.00	0.00	3A7
ATOM	1233	СВ	ASN	198	37.878 -	12.191	34.815	1.00	0.00	3A7
ATOM	1234	CG	ASN	198	37.631 -	11.423	36.121	1.00	0.00	3A7
MOTA	1235	OD1	ASN	198	37.872 -		37.214	1.00	0.00	3A7
MOTA	1236	ND2	ASN	198	37.143 -		35.986	1.00	0.00	3A7
ATOM	1237	С	ASN	198	36.725 -		32.825	1.00	0.00	3A7
ATOM	1238	0	ASN	198	36.624 -		31.789	1.00	0.00	3A7
MOTA	1239	N	PRO		36.993 -		32.735	1.00	0.00	3A7
ATOM	1240	CA	PRO		37.251 -		31.473	1.00		3A7 3A7
ATOM	1241 1242	CD	PRO		37.339 - 37.966 -		33.865 31.866	1.00		3A7
ATOM		CB CG	PRO		38.421 -		33.313	1.00		3A7
ATOM ATOM	1243 1244	C	PRO PRO		35.959 -		30.731	1.00		3A7
ATOM	1244	Ö	PRO		36.016 -		29.524	1.00		3A7
ATOM	1246	N	GLN		34.800 -		31.441	1.00		3A7
ATOM	1247	CA	GLN		33.519 -		30.914	1.00		3A7
ATOM	1248	СВ	GLN		32.614 -		32.023	1.00		3A7
ATOM	1249	CG	GLN		31.297 -		31.515	1.00		3A7
ATOM	1250	CD	GLN		30.581 -		32.668			3A7
MOTA	1251		GLN		30.411 -		32.645			3A7
ATOM	1252	NE2	GLN	200	30.150 -	17.085	33.690	1.00	0.00	3A7

ATOM	1253	С	GLN	200	32.815 -	14.819	30.232	1.00	0.00	3A7
ATOM	1254	0	GLN	200	32.140 -		29.233	1.00	0.00	3A7
MOTA	1255	N	ASP	201	32.961 -		30.743	1.00	0.00	3A7
ATOM	1256	CA	ASP	201	32.288 -		30.219	1.00	0.00	3A7
MOTA	1257	CB	ASP	201	32.223 -		31.288	1.00	0.00	3A7 3A7
ATOM	1258	CG	ASP	201	31.197 -		30.927 30.772	1.00	0.00 0.00	3A7
MOTA	1259	OD1		201 201	31.610 29.992 -		30.772	1.00	0.00	3A7
ATOM ATOM	1260 1261	OD2 C	ASP	201	32.876 -		28.899	1.00	0.00	3A7
ATOM	1262	ŏ	ASP	201	32.107 -		28.095	1.00	0.00	3A7
ATOM	1263	N	PRO	202	34.177 -		28.590	1.00	0.00	3A7
ATOM	1264	CA	PRO	202	34.768 -		27.282	1.00	0.00	3A7
ATOM	1265	CD	PRO	202	35.191 -	11.898	29.612	1.00	0.00	3A7
MOTA	1266	СВ	PRO	202	36.280 -	11.790	27.543	1.00	0.00	3A7
ATOM	1267	CG	PRO	202	36.411 -		28.958	1.00	0.00	3A7
ATOM	1268	С	PRO	202	34.334 -		26.270	1.00	0.00	3A7
MOTA	1269	0	PRO	202	34.099 -		25.126	1.00	0.00	3A7
MOTA	1270	N	PHE	203	34.165 -		26.662	1.00	0.00	3A7 3A7
ATOM	1271	CA	PHE	203	33.692 - 33.533 -		25.807 26.628	1.00	0.00	3A7
ATOM ATOM	1272 1273	CB CG	PHE	203 203	33.530 -		25.800	1.00	0.00	3A7
ATOM	1273		PHE	203	34.701 -		25.685	1.00	0.00	3A7
ATOM	1275		PHE	203	32.364 -		25.192	1.00	0.00	3A7
ATOM	1276		PHE	203	34.713 -		24.981	1.00	0.00	3A7
ATOM	1277		PHE	203	32.377 -		24.471	1.00	0.00	3A7
ATOM	1278	CZ	PHE	203	33.547 -	-20.060	24.377	1.00	0.00	3A7
ATOM	1279	С	PHE	203	32.360 -	-14.780	25.173	1.00	0.00	3A7
ATOM	1280	0	PHE	203	32.125 -		23.999	1.00	0.00	3A7
MOTA	1281	N	VAL	204	31.455 -		25.959	1.00	0.00	3A7
ATOM	1282	CA	VAL	204	30.141 -		25.564	1.00	0.00	3A7
MOTA	1283	CB	VAL	204	29.470 -		26.710	1.00	0.00	3A7 3A7
ATOM	1284		VAL VAL	204	28.141 - 29.308 -		26.286 27.927	1.00 1.00	0.00	3A7
ATOM ATOM	1285 1286	C	VAL	204 204	30.210		24.430	1.00	0.00	3A7
ATOM	1287	ō	VAL	204	29.521		23.424	1.00	0.00	3A7
ATOM	1288	N	GLU	205	31.077		24.576	1.00	0.00	3A7
ATOM	1289	CA	GLU	205	31.235		23.617	1.00	0.00	3A7
ATOM	1290	СВ	GLU	205	32.215	-9.544	24.146	1.00	0.00	3A7
ATOM	1291	CG	GLU	205	32.242	-8.242	23.327	1.00	0.00	3A7
MOTA	1292	CD	GLU	205	33.217	-7.267	23.979	1.00	0.00	3A7
ATOM	1293		GLU	205	32.974	-6.880	25.153	1.00	0.00	3A7
ATOM	1294		GLU	205	34.219	-6.896	23.310	1.00	0.00	3A7
MOTA	1295	C	GLU	205	31.739		22.289	1.00	0.00	3A7 3A7
ATOM	1296	0	GLU	205 206	31.308 32.629		21.238 22.316	1.00	0.00	3A7
ATOM ATOM	1297 1298	N CA	ASN ASN	206	33.175		21.134	1.00	0.00	3A7
ATOM	1299	СВ	ASN	206	34.358		21.467	1.00	0.00	3A7
ATOM	1300	ĊĠ	ASN	206	35.509		22.025	1.00	0.00	3A7
ATOM	1301		ASN	206	35.798	-12.848	23.224	1.00	0.00	. 3A7
ATOM	1302	ND2	ASN	206	36.155	-12.023	21.120	1.00	0.00	3A7
MOTA	1303	С	ASN	206		-13.539	20.380	1.00	0.00	3A7
MOTA	1304	0	ASN	206		-13.337	19.182	1.00	0.00	3A7
ATOM	1305	N	THR	207		-14.452	21.067	1.00	0.00	3A7
ATOM	1306	CA	THR	207		-15.301	20.464	1.00 1.00	0.00	3A7 3A7
ATOM	1307 1308	CB	THR THR			-16.188 -16.917	21.502 22.199	1.00	0.00	3A7
ATOM ATOM	1308		THR			-17.201	20.851	1.00	0.00	3A7
ATOM	1310	C	THR			-14.492	19.768	1.00	0.00	3A7
ATOM	1311	ŏ	THR			-14.790	18.646	1.00	0.00	3A7
ATOM	1312	N	LYS			-13.379	20.411	1.00	0.00	3A7
ATOM	1313	CA	LYS			-12.459	19.890	1.00	0.00	3A7
MOTA	1314	СВ	LYS			-11.413	20.954	1.00	0.00	3A7
ATOM	1315	CG	LYS			-10.524	20.601	1.00	0.00	3A7
ATOM	1316	CD	LYS		25.914	-9.608	21.741	1.00	0.00	3A7
ATOM	1317	CE	LYS		26.801	-8.383	22.018	1.00	0.00	3A7
MOTA	1318	NZ	LYS		28.077	-8.751	22.673	1.00	0.00	3A7 3A7
ATOM	1319	C	LYS			-11.760 -11.653	18.619 17.675	1.00	0.00	3A7
MOTA MOTA	1320 1321	O N	LYS LYS			-11.833	18.536			3A7
ATOM	1321	CA	LYS			-10.686	17.348			3A7
ATOM	1323	CB	LYS			-10.129	17.587			3A7
ATOM	1324	CG	LYS		31.660	-8.877	18.478			3A7
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MOTA	1325	CD	LYS	209	33.007	-8.133	18.418	1.00	0.00	3A7
ATOM	1326	CE	LYS	209	34.227	-8.963	18.843	1.00	0.00	3A7
ATOM	1327	NZ	LYS	209	34.144	-9.343	20.270	1.00	0.00	3A7 3A7
ATOM	1328 1329	С 0	LYS LYS	209 209		-11.624 -11.252	16.153 15.031	1.00	0.00	3A7
ATOM ATOM	1330	N	LEU	210		-12.901	16.376	1.00	0.00	3A7
ATOM	1331	CA	LEU	210		-13.968	15.391	1.00	0.00	3A7
ATOM	1332	СВ	LEU	210	30.985	-15.328	16.011	1.00	0.00	3A7
MOTA	1333	CG	LEU	210		-16.622	15.108	1.00	0.00	3A7
MOTA	1334	CD1		210		-17.872	16.013	1.00	0.00	3A7 3A7
ATOM	1335	CD2		210		-16.893 -14.131	13.954 14.809	1.00	0.00	3A7
ATOM ATOM	1336 1337	С 0	LEU	210 210		-14.197	13.595	1.00	0.00	3A7
ATOM	1338	N	LEU	211		-14.172	15.680	1.00	0.00	3A7
ATOM	1339	CA	LEU	211	26.814	-14.406	15.302	1.00	0.00	3A7
MOTA	1340	СВ	LEU	211		-14.273	16.480	1.00	0.00	3A7
ATOM	1341	CG	LEU	211		-15.159	17.726	1.00	0.00	3A7
ATOM	1342		LEU	211		-15.056 -16.614	18.669 17.396	1.00	0.00	3A7 3A7
ATOM ATOM	1343 1344	CD2	LEU LEU	211 211		-13.442	14.274	1.00	0.00	3A7
ATOM	1345	Ö	LEU	211		-13.847	13.418	1.00	0.00	3A7
ATOM	1346	N	ARG	212		-12.140	14.324	1.00	0.00	3A7
MOTA	1347	CA	ARG	212	26.196	-11.136	13.386	1.00	0.00	3A7
MOTA	1348	CB	ARG	212	25.985		14.028	1.00	0.00	3A7
ATOM	1349	CG	ARG	212	27.103		14.927	1.00	0.00 0.00	3A7 3A7
ATOM	1350	CD	ARG ARG	212	28.270 29.078		14.183 15.175	1.00	0.00	3A7
ATOM ATOM	1351 1352	NE CZ	ARG	212 212	30.393		14.970	1.00	0.00	3A7
ATOM	1353		ARG	212	31.075		13.898	1.00	0.00	3A7
ATOM	1354		ARG	212	31.031		15.851	1.00	0.00	3A7
ATOM	1355	С	ARG	212		-11.091	12.169	1.00	0.00	3A7
ATOM	1356	0	ARG	212		-11.083	12.272	1.00	0.00	3A7
ATOM	1357	N	PHE	213		-11.117	10.976 9.611	1.00	0.00	3A7 3A7
ATOM	1358 1359	CA CB	PHE	213 213	26.943	-11.263	8.921	1.00	0.00	3A7
ATOM ATOM	1360	CG	PHE	213	28.597		9.541	1.00	0.00	3A7
ATOM	1361		PHE	213	28.391		10.535	1.00	0.00	3A7
ATOM	1362	CD2	PHE	213	29.890	-9.399	9.039	1.00	0.00	3A7
MOTA	1363		PHE	213	29.455		11.032	1.00	0.00	3A7
ATOM	1364		PHE	213	30.959		9.546 10.544	1.00	0.00	3A7 3A7
ATOM ATOM	1365 1366	CZ C	PHE	213 213	30.741	-12.408	9.426	1.00	0.00	3A7
MOTA	1367	ŏ	PHE	213		-12.215	9.209	1.00	0.00	3A7
ATOM	1368	N	ASN	214		-13.649	9.491	1.00	0.00	3A7
ATOM	1369	CA	ASN	214	28.142	2 -14.839	9.165	1.00	0.00	3A7
MOTA	1370	CB	ASN	214		-15.372	10.314	1.00	0.00	3A7
ATOM	1371	CG	ASN	214		-16.484	9.818 8.972	1.00	0.00	3A7 3A7
ATOM ATOM	1372		ASN ASN	214 214		3 -16.242 3 -17.720	10.370	1.00	0.00	3A7
ATOM	1374	C	ASN	214		-15.863	8.671	1.00	0.00	3A7
ATOM	1375	ō	ASN	214		5 -16.351	7.565	1.00	0.00	3A7
ATOM	1376	N	PRO	215		-16.260		1.00	0.00	3A7
ATOM	1377	CA	PRO	215		0 -17.305		1.00	0.00	3A7 3A7
MOTA	1378	CD	PRO	215		9 - 15.929 6 -17.865		1.00	0.00	3A7
MOTA MOTA	1379 1380	CB CG	PRO PRO	215 215		6 -17.863 6 -17.241		1.00	0.00	3A7
ATOM	1381	c	PRO	215		8 -16.681		1.00	0.00	3A7
ATOM	1382	O	PRO	215		6 -15.982	8.353	1.00	0.00	3A7
ATOM	1383	N	LEU	216		3 ~16.921		1.00	0.00	3A7
ATOM	1384	CA	LEU	216		6 -16.424			0.00	3A7 3A7
ATOM	1385	CB	LEU	216		1 -16.737 9 -19 22 <i>4</i>			0.00	3A7
MOTA MOTA	1386 1387	CC	LEU LEU	216 216		9 -18.224 0 -18.782				3A7
ATOM	1388		LEU LEU	216		2 -19.148				3A7
ATOM	1389	c c	LEU	216		3 -14.925	5.304	1.00	0.00	3A7
ATOM	1390	0	LEU	216		6 -14.143				3A7
ATOM	1391	N	ASP	217		1 -14.501				3A7
ATOM	1392	CA	ASP	217		2 -13.102 6 -12.608				3A7 3A7
ATOM	1393	CB CG	ASP ASP	217 217		5 -12.608 5 -13.427				3A7
ATOM ATOM	1394 1395		ASP 1 ASP			8 -12.833				3A7
ATOM	1396		2 ASP			0 -14.641				3A7

ATOM	1397	С	ASP	217	25.056	-12.846	2.709	1.00	0.00	3A7
ATOM	1398	ō	ASP	217	26.126		2.166	1.00	0.00	3A7
ATOM	1399	N	PRO	218	24.053		2.013	1.00	0.00	3A7
ATOM	1400	CA	PRO	218	24.193		0.691	1.00	0.00	3A7
ATOM	1401	CD	PRO	218	22.655		2.382	1.00	0.00	3A7
ATOM	1402	СВ	PRO	218	22.746		0.203	1.00	0.00	3A7
		CG	PRO	218	21.908		1.050	1.00	0.00	3A7
ATOM	1403				24.945		0.782	1.00	0.00	3A7
ATOM	1404	C	PRO	218			1.833	1.00	0.00	3A7
ATOM	1405	0	PRO	218	24.911	-9.730		1.00	0.00	3A7
ATOM	1406	N	PHE	219	25.621	-9.950	-0.316			
ATOM	1407	CA	PHE	219	26.432	-8.745	-0.344	1.00	0.00	3A7
MOTA	1408	СВ	PHE	219	27.591	-8.800	-1.373	1.00	0.00	3A7
MOTA	1409	CG	PHE	219	28.495	-9.952	-1.047	1.00	0.00	3A7
ATOM	1410		PHE	219	29.296	-9.917	0.094	1.00	0.00	3A7
ATOM	1411	CD2	PHE	219	28.551	-11.070	-1.881	1.00	0.00	3A7
MOTA	1412	CEI	PHE	219	30.140		0.400	1.00	0.00	3A7
ATOM	1413	CE2	PHE	219	29.393	-12.136	-1.578	1.00	0.00	3A7
ATOM	1414	CZ	PHE	219	30.189	-12.092	-0.437	1.00	0.00	3A7
ATOM	1415	Ç	PHE	219	25.587	-7.501	-0.570	1.00	0.00	3A7
ATOM	1416	O	PHE	219	25.626	-6.607	0.273	1.00	0.00	3A7
ATOM	1417	N	VAL	220	24.790	-7.366	-1.669	1.00	0.00	3A7
ATOM	1418	CA	VAL	220	24.617	-8.245	-2.807	1.00	0.00	3A7
ATOM	1419	СВ	VAL	220	23.148	-8.591	-3.051	1.00	0.00	3A7
ATOM	1420		VAL	220	22.271	-7.323	-3.127	1.00	0.00	3A7
				220	22.991	-9.517	-4.277	1.00	0.00	3A7
ATOM	1421		VAL		25.287	-7.570	-3.983	1.00	0.00	3A7
MOTA	1422	C	VAL	220		-8.235	-4.883	1.00	0.00	3A7
MOTA	1423	0	VAL	220	25.799	-6.211		1.00	0.00	3A7
ATOM	1424	N	LEU	221	25.336		~3.963			3A7
ATOM	1425	CA	LEU	221	26.163	-5.403	-4.835	1.00	0.00	
ATOM	1426	CB	LEU	221	25.390	-4.284	-5.597	1.00	0.00	3A7
ATOM	1427	CG	LEU	221	24.479	-4.750	-6.764	1.00	0.00	3A7
MOTA	1428		LEU	221	25.258	-5.539	-7.835	1.00	0.00	3A7
ATOM	1429		LEU	221	23.213	-5.501	-6.317	1.00	0.00	3A7
ATOM	1430	¢	LEU	221	27.196	-4.792	-3.913	1.00	0.00	3A7
ATOM	1431	0	LEU	221	27.565	-5.391	-2.904	1.00	0.00	3A7
MOTA	1432	N	SER	222	27.682	-3.567	-4.239	1.00	0.00	3A7
ATOM	1433	CA	SER	222	28.622	-2.816	-3.435	1.00	0.00	3A7
ATOM	1434	СВ	SER	222	29.722	-2.139	-4.284	1.00	0.00	3A7
MOTA	1435	OG	SER	222	30.472	-3.121	-4.985	1.00	0.00	3A7
ATOM	1436	С	SER	222	27.841	-1.762	-2.698	1.00	0.00	3A7
ATOM	1437	0	SER	222	27.764	-0.612	-3.127	1.00	0.00	3A7
ATOM	1438	N	ILE	223	27.222	-2.164	-1.561	1.00	0.00	3A7
ATOM	1439	CA	ILE	223	26.322	-1.338	-0.788	1.00	0.00	3A7
ATOM	1440	СВ	ILE	223	24.971	-2.017	-0.555	1.00	0.00	3A7
ATOM	1441		ILE	223	25.156	-3.487	-0.110	1.00	0.00	3A7
ATOM	1442		ILE	223	24.042	-1.193	0.374	1.00	0.00	3A7
ATOM	1443	CD.	ILE	223	22.603	-1.718	0.416	1.00	0.00	3A7
ATOM	1444	c	ILE	223	27.019	-0.926	0.488	1.00	0.00	3A7
MOTA	1445	Ö	ILE	223	27.093	0.266	0.787	1.00	0.00	3A7
ATOM	1446	N	LYS	224	27.556	-1.893	1.271	1.00	0.00	3A7
ATOM	1447	CA	LYS	224	28.263	-1.581	2.490	1.00	0.00	3A7
	1448	CB	LYS	224	27.339	-1.185	3.674	1.00	0.00	3A7
ATOM	1449			224	28.088	-0.528	4.849	1.00	0.00	3A7
ATOM		CG	LYS		27.190	-0.187	6.049	1.00	0.00	3A7
MOTA	1450	CD	LYS	224			6.861	1.00	0.00	3A7
ATOM	1451	CE	LYS	224	26.740	-1.411				
MOTA	1452	NZ	LYS	224	27.901	-2.112	7.458	1.00	0.00	3A7
ATOM	1453	С	LYS	224	29.052		2.890	1.00	0.00	3A7
MOTA	1454	0	LYS	224	30.070		3.572		0.00	3A7
ATOM	1455	Ŋ	VAL	225	28.582		2.483		0.00	3A7
ATOM	1456	CA	VAL	225	29.124		2.907		0.00	3A7
ATOM	1457	СВ	VAL	225	28.125		2.746		0.00	3A7
MOTA	1458		l VAL	225	28.683		3.365		0.00	3A7
ATOM	1459	CG	2 VAL	225	26.805		3.429		0.00	3A7
ATOM	1460	С	VAL	225	30.398	-5.583	2.147	1.00		3A7
ATOM	1461	0	VAL	225	31.486	-5.449	2.708	1.00	0.00	3A7
ATOM	1462	N	PHE	226	30.271		0.851	1.00	0.00	3A7
ATOM	1463	CA	PHE	226	31.349		-0.106		0.00	3A7
ATOM	1464	CB	PHE		32.367		-0.098			3A7
ATOM	1465	CG	PHE	226	33.203		-1.346			3A7
ATOM	1466		1 PHE		34.585		-1.283			3A7
ATOM	1467		2 PHE		32.615		-2.578			3A7
ATOM	1468		2 PAE 1 PHE		35.365		-2.432			3A7
A I OU	1400	ÇE		220	55.555	5.025	~. · · · · · ·			

MOTA	1469	CE2	PHE	226	33.393	-4.550	-3.730	1.00	0.00	3A7
ATOM	1470	CZ	PHE	226	34.768	-4.749	-3.658	1.00	0.00	3A7
ATOM	1471	C	PHE	226	32.059	-7.514	0.144	1.00	0.00	3A7
ATOM	1472	ō	PHE	226	32.151	-7.943	1.295	1.00	0.00	3A7
ATOM	1473	N	PRO	227	32.610	-8.198	-0.871	1.00	0.00	3A7
ATOM	1474	CA	PRO	227	33.431	-9.392	-0.698	1.00	0.00	3A7
ATOM		CD	PRO	227	32.111	-8.089	-2.237	1.00	0.00	3A7
	1475			227	33.602	-9.944	-2.123	1.00	0.00	3A7
MOTA	1476	СВ	PRO		32.349	-9.465	-2.857	1.00	0.00	3A7
ATOM	1477	CG	PRO	227			-0.061	1.00	0.00	3A7
ATOM	1478	C	PRO	227	34.778	-9.081		1.00	0.00	3A7
MOTA	1479	0	PRO	227	35.140	-7.911	0.062		0.00	3A7
ATOM	1480	N	PHE	228		-10.132	0.346	1.00		3A7
MOTA	1481	CA	PHE	228		-10.004	1.060	1.00	0.00	
MOTA	1482	CB	PHE	228		-11.255	1.926	1.00	0.00	3A7
MOTA	1483	CG	PHE	228		-12.560	1.172	1.00	0.00	3A7
MOTA	1484	CD1	PHE	228		-13.176	0.937	1.00	0.00	3A7
ATOM	1485	CD2	PHE	228	38.217	-13.193	0.733	1.00	0.00	3A7
ATOM	1486	CE1	PHE	228	35.753	-14.388	0.257	1.00	0.00	3A7
MOTA	1487	CE2	PHE	228	38.152	-14.405	0.053	1.00	0.00	3A7
ATOM	1488	CZ	PHE	228	36.919	-15.003	-0.187	1.00	0.00	3A7
ATOM	1489	С	PHE	228	37.924	-9.676	0.107	1.00	0.00	3A7
ATOM	1490	ō	PHE	228	38.323	-10.488	-0.727	1.00	0.00	3A7
ATOM	1491	N	LEU	229	38.440	-8.432	0.225	1.00	0.00	3A7
ATOM	1492	CA	LEU	229	39.469	-7.914	-0.636	1.00	0.00	3A7
	1493	CB	LEU	229	38.924	-7.440	-2.010	1.00	0.00	3A7
ATOM		CG	LEU	229	39.979	-6.871	-2.990	1.00	0.00	3A7
ATOM	1494				41.083	-7.892	-3.326	1.00	0.00	3A7
ATOM	1495		LEU	229	39.305	-6.347	-4.273	1.00	0.00	3A7
ATOM	1496		LEU	229			0.105	1.00	0.00	3A7
MOTA	1497	C	LEU	229	40.062	-6.752			0.00	3A7
MOTA	1498	0	LEU	229	41.281	-6.639	0.226	1.00	0.00	3A7
MOTA	1499	N	THR	230	39.186	-5.847	0.615	1.00		3A7
MOTA	1500	CA	THR	230	39.568	-4.636	1.308	1.00	0.00	
ATOM	1501	CB	THR	230	38.715	-3.444	0.870	1.00	0.00	3A7
ATOM	1502	OG1	THR	230	39.184	-2.215	1.417	1.00	0.00	3A7
ATOM	1503	CG2	THR	230	37.220	-3.639	1.206	1.00	0.00	3A7
MOTA	1504	С	THR	230	39.476	-4.902	2.807	1.00	0.00	3A7
MOTA	1505	0	THR	230	38.513	-5.527	3.250	1.00	0.00	3A7
ATOM	1506	N	PRO	231	40.435	-4.450	3.626	1.00	0.00	3A7
ATOM	1507	CA	PRO	231	40.382	-4.534	5.074	1.00	0.00	3A7
ATOM	1508	CD	PRO	231	41.737	-3.996	3.151	1.00	0.00	3A7
ATOM	1509	СВ	PRO	231	41.866	-4.556	5.472	1.00	0.00	3A7
ATOM	1510	CG	PRO	231	42.555	-3.696	4.409	1.00	0.00	3A7
ATOM	1511	c	PRO	231	39.661	-3.313	5.625	1.00	0.00	3A7
ATOM	1512	ō	PRO	231	38.946		4.885	1.00	0.00	3A7
ATOM	1513	N	ILE	232	39.877		6.939	1.00	0.00	3A7
ATOM	1514	CA	ILE	232	39.462		7.738	1.00	0.00	3A7
ATOM	1515	CB	ILE	232	40.410		7.563	1.00	0.00	3A7
	1516	CG2		232	40.450		6.123	1.00	0.00	3A7
ATOM					40.186		8,608	1.00	0.00	3A7
ATOM	1517	CGI		•			10.038	1.00	0.00	3A7
ATOM	1518	CD	ILE	232	40.563		7.610	1.00	0.00	3A7
ATOM	1519	С	ILE	232	37.983		6.949	1.00	0.00	3A7
ATOM	1520	0	ILE	232	37.631			1.00	0.00	3A7
ATOM	1521	N	LEU	233	37.047		8.259			3A7
MOTA	1522	CA	LEU	233	37.231		8.977	1.00	0.00	3A7
MOTA	1523	СВ	LEU	233	36.638			1.00		
ATOM	1524	CG	LEU	233	37.361			1.00		3A7
MOTA	1525	CD:	L LEU	233	38.832					3A7
ATOM	1526	CD	2 LEU	233	37.198					3A7
MOTA	1527	С	LEU	233	36.518	-4.523	8.138			3A7
ATOM	1528	0	LEU	233	36.754	-4.608	6.933	1.00	0.00	3A7
MOTA	1529	N	GLU	234	35.621	-5.330	8.775	1.00	0.00	3A7
ATOM	1530		GLU		34.755	-6.337	8.183	1.00	0.00	3A7
MOTA	1531		GLU		33.985			1.00	0.00	3A7
ATOM	1532		GLU		32.750				0.00	3A7
ATOM	1533		GLU		33.14					3A7
ATOM	1534		1 GLU		33.79					3A7
ATOM	1535		2 GLU		32.78					3A7
			GLU		35.545					3A7
MOTA	1536				36.38					3A7
ATOM	1537		GLU		35.26					3A7
MOTA	1538		ALA			7 -0.001 3 -10.014				3A7
ATOM	1539					9 -10.014 9 -10.390				3A7
MOTA	1540	СВ	ALA	235	30.26	, -1U.37U	, ,			J

										27.7
MOTA	1541		ALA	235		-10.214	9.409		0.00 0.00	3A7 3A7
ATOM	1542	0	ALA	235	-	-11.312	9.899		0.00	3A7
MOTA	1543	N	LEU	236	37.790	-9.141	9.671 10.503		0.00	3A7
MOTA	1544	CA	LEU	236	38.971	-9.206	10.361		0.00	3A7
MOTA	1545	CB	LEU	236	39.828 40.242	-7.935 -7.612	8.906		0.00	3A7
MOTA	1546 1547	CG	LEU	236 236	40.242	-6.254	8.836	1.00	0.00	3A7
ATOM	1547	CD1 CD2		236	41.094	-8.728	8.272	1.00	0.00	3A7
MOTA MOTA	1549	C	LEU	236	38.601	-9.366	11.956	1.00	0.00	3A7
ATOM	1550	ō	LEU	236	39.204		12.697	1.00	0.00	3A7
ATOM	1551	N	ASN	237	37.530		12.387	1.00	0.00	3A7
ATOM	1552	CA	ASN	237	37.020		13.741	1.00	0.00	3A7
ATOM	1553	СВ	ASN	237	35.917		13.982	1.00	0.00	3A7
ATOM	1554	CG	ASN	237	36.463		13.746	1.00	0.00	3A7
ATOM	1555	OD1	ASN	237	35.922	-5.526	12.923	1.00	0.00	3A7
ATOM	1556	ND2	ASN	237	37.544		14.500	1.00	0.00	3A7
ATOM	1557	С	ASN	237		-10.107	14.022	1.00	0.00	3A7
MOTA	1558	0	ASN	237		-10.658	15.111	1.00	0.00	3A7
ATOM	1559	N	ILE	238		-10.707	12.979	1.00	0.00	3A7 3A7
MOTA	1560	CA	ILE	238		-12.011	13.021	1.00	0.00	3A7
MOTA	1561	CB	ILE	238		-12.290	11.743	1.00	0.00	3A7
MOTA	1562		ILE	238		1 -13.648	11.845 11.432	1.00	0.00	3A7
MOTA	1563		ILE	238		-11.141 7 -10.932	12.495	1.00	0.00	3A7
ATOM	1564	CD	ILE	238) -13.064	13.260	1.00	0.00	3A7
MOTA MOTA	1565 1566	С 0	ILE	238 238		-13.896	14.106	1.00	0.00	3A7
ATOM	1567	N	THR	239		2 -13.013	12.556	1.00	0.00	3A7
ATOM	1568	CA	THR	239		5 -13.929	12.699	1.00	0.00	3A7
ATOM	1569	CB	THR	239		6 -13.767	11.574	1.00	0.00	3A7
ATOM	1570		THR	239		-13.766	10.323	1.00	0.00	3A7
ATOM	1571	CG2	THR	239	40.562	2 -14.928	11.571	1.00	0.00	3A7
MOTA	1572	С	THR	239		6 -13.773	14.033	1.00	0.00	3A7
ATOM	1573	0	THR	239		0 -14.740	14.603	1.00	0.00	3A7 3A7
ATOM	1574	N	VAL	240		4 -12.555	14.619	1.00	0.00	3A7
ATOM	1575	CA	VAL VAL	240 240		9 -12.276 0 -10.784	15.932 16.162	1.00	0.00	3A7
ATOM ATOM	1576 1577	CB	VAL	240		6 -10.421	17.627	1.00	0.00	3A7
ATOM	1578		VAL	240		6 -10.316	15.239	1.00	0.00	3A7
ATOM	1579	c	VAL	240		1 -12.842	17.025	1.00	0.00	3A7
ATOM	1580	0	VAL	240	39.41	8 -13.460	17.956	1.00	0.00	3A7
MOTA	1581	N	PHE	241		8 -12.667	16.920	1.00	0.00	3A7
MOTA	1582	CA	PHE	241		4 -13.266	17.837	1.00	0.00	3A7
ATOM	1583	СВ	PHE	241		0 -12.893	17.483	1.00	0.00 0.00	3A7 3A7
ATOM	1584	CG	PHE	241		2 -14.041 8 -15.104	17.098 17.973	1.00	0.00	3A7
MOTA	1585		PHE	241 241		8 -14.250	15.746	1.00	0.00	3A7
ATOM ATOM	1586 1587		PHE	241		1 -16.400	17.483	1.00	0.00	3A7
ATOM	1588		PHE	241		6 -15.545	15.244	1.00	0.00	3A7
ATOM	1589	ÇZ	PHE	241		8 -16.626	16.119	1.00	0.00	. 3A7
ATOM	1590	Ċ	PHE	241	36.78	4 -14.763	17.938	1.00	0.00	3A7
MOTA	1591	0	PHE	241		7 -15.276	19.050	1.00	0.00	3A7
MOTA	1592	N	PRO	242		3 -15.511		1.00	0.00	3A7
MOTA	1593	CA	PRO	242		2 -16.902	16.784	1.00	0.00	3A7 3A7
ATOM	1594	CD	PRO	242		7 ~15.196			0.00	3A7
ATOM	1595	CB	PRO	242		15 -17.375 13 -16.221				3A7
MOTA MOTA	1596 1597	CG C	PRO PRO	242 242		14 -17.310				3A7
MOTA	1598	Ö	PRO	242		1 -18.268				3A7
ATOM	1599	N	ARG	243		9 -16.603				3A7
ATOM	1600	CA	ARG	243		1 -16.892			0.00	3A7
ATOM	1601	CB	ARG	243	41.73	34 -15.942	17.355	1.00		3A7
ATOM	1602	CG	ARG	243	42.17	72 -16.265				3A7
MOTA	1603	ÇD	ARG	243		02 -15.187				3A7
ATOM	1604	NE	ARG	243		25 -15.532				3A7 3A7
ATOM	1605	CZ	ARG	243		62 -14.651				3A7 3A7
ATOM	1606		1 ARG	243		10 -15.003 44 -13.422				3A7
ATOM	1607		2 ARG ARG	243 243		94 -13.422 82 -16.769				3A7
MOTA MOTA	1608 1609		ARG			52 -17.580				3A7
ATOM	1610		LYS			13 -15.774				3A7
ATOM	1611					42 -15.565	21.32	7 1.00		3A7
ATOM	1612				39.0	46 -14.178	3 21.648	3 1.00	0.00	3A7

ATOM	1613	CG	LYS	244	39.241 - 13.	772 23.119	1.00	0.00	3A7
ATOM	1614	CD	LYS	244	39.058 -12.	271 23.402	1.00	0.00	3A7
MOTA	1615	CE	LYS	244	40.110 -11.		1.00	0.00	3A7
ATOM	1616	NZ	LYS	244	41.474 -11.		1.00	0.00	3A7
ATOM	1617	С	LYS	244	38.844 -16.		1.00	0.00	3A7
MOTA	1618	0	LYS	244	39.175 -17.		1.00	0.00	3A7
ATOM	1619	N	VAL	245	37.806 -17.		1.00	0.00	3A7 3A7
ATOM	1620	CA	VAL	245	37.014 -18. 35.821 -18.		1.00	0.00	3A7
ATOM	1621	CB	VAL	245 245	35.055 -19.		1.00	0.00	3A7
MOTA MOTA	1622 1623		VAL VAL	245	34.893 -17.		1.00	0.00	3A7
ATOM	1624	C	VAL	245	37.868 -19.		1.00	0.00	3A7
ATOM	1625	ŏ	VAL	245	37.867 -20.		1.00	0.00	3A7
ATOM	1626	N	ILE	246	38.674 -19.		1.00	0.00	3A7
ATOM	1627	CA	ILE	246	39.563 -20.	965 20.600	1.00	0.00	3A7
ATOM	1628	CB	ILE	246	40.252 -21.	026 19.232	1.00	0.00	3A7
ATOM	1629	CG2	ILE	246	41.696 -21.		1.00	0.00	3A7
MOTA	1630	CG1	ILE	246	39.414 -21.		1.00	0.00	3A7
ATOM	1631	CD	ILE	246	38.083 -21.		1.00	0.00	3A7
MOTA	1632	C	ILE	246	40.571 -20.		1.00	0.00	3A7
ATOM	1633	0	ILE	246	40.828 -21.		1.00	0.00 0.00	3A7 3A7
ATOM	1634	N	SER	247	41.133 -19. 42.119 -19.		1.00 1.00	0.00	3A7
ATOM	1635	CA	SER	247	42.734 -18		1.00	0.00	3A7
ATOM	1636 1637	CB OG	SER SER	247 247	43.425 -18		1.00	0.00	3A7
ATOM ATOM	1638	C	SER	247	41.551 -19		1.00	0.00	3A7
ATOM	1639	o	SER	247	42.194 -20		1.00	0.00	3A7
ATOM	1640	N	PHE	248	40.320 -19		1.00	0.00	3A7
ATOM	1641	CA	PHE	248	39.670 -19		1.00	0.00	3A7
ATOM	1642	CB	PHE	248	38.328 -18	.900 26.125	1.00	0.00	3A7
ATOM	1643	ÇG	PHE	248	38.514 -17	.473 26.559	1.00	0.00	3A7
ATOM	1644	CD1	PHE	248	37.951 - 16		1.00	0.00	. 3A7
ATOM	1645	CD2	PHE	248	39.191 -17		1.00	0.00	3A7
ATOM	1646		PHE	248	38.058 -15		1.00	0.00	3A7
MOTA	1647		PHE	248	39.316 -15		1.00	0.00	3A7 3A7
ATOM	1648	CZ	PHE	248	38.749 -14		1.00	0.00 0.00	3A7
ATOM	1649	C	PHE	248	39.389 -21 39.623 -21		1.00	0.00	3A7
ATOM	1650	O N	PHE	248 249	38.919 -21		1.00	0.00	3A7
ATOM ATOM	1651 1652	CA	LEU	249	38.585 -23		1.00	0.00	3A7
ATOM	1653	СВ	LEU	249	37.717 -23		1.00	0.00	3A7
ATOM	1654	CG	LEU	249	36.376 -22		1.00	0.00	3A7
ATOM	1655		LEU	249	35.616 -23		1.00	0.00	3A7
ATOM	1656	CD2	LEU	249	35.503 -23	.243 25.342	1.00	0.00	3A7
ATOM	1657	С	LEU	249	39.811 -24			0.00	3A7
MOTA	1658	0	LEU	249	39.841 -25			0.00	3A7
ATOM	1659	N	THR	250	40.891 -23			0.00	3A7
ATOM	1660	CA	THR	250	42.150 -24			0.00	3A7 3A7
ATOM	1661	СВ	THR	250	43.131 -23			0.00	3A7
ATOM	1662		THR	250 250	42.595 -24 44.496 - 24			0.00	3A7
ATOM ATOM	1663 1664	C	THR THR	250	42.765 -24			0.00	3A7
ATOM	1665	ò	THR	250	43.326 -25				3A7
ATOM	1666	N	LYS	251	42.622 -23				3A7
ATOM	1667	CA	LYS	251	43.087 -23				3A <u>7</u>
ATOM	1668	СВ	LYS	251	42.941 -21		1.00	0.00	3A7
ATOM	1669	CG	LYS	251	43.599 -21	.282 29.945	1.00		3A7
ATOM	1670	CD	LYS	251	43.466 -19				3A7
ATOM	1671	CE	LYS	251	44.093 -19				3A7
MOTA	1672	NZ	LYS	251	43.930 -18				3A7
MOTA	1673	C	LYS		42.337 -23				3A7
ATOM	1674	0	LYS		42.946 -24				3A7 3A7
ATOM	1675	N	SER		40.996 -24 40.169 -24				3A7 3A7
MOTA	1676	CA	SER		40.169 -24 38.679 -24				3A7 3A7
ATOM ATOM	1677 1678	CB OG	SER SER		38.257 -23				3A7
ATOM	1678	C	SER		40.543 -20				3A7
ATOM	1680	0	SER		40.637 -2				3A7
ATOM	1681	N	VAL		40.836 -20				3A7
ATOM	1682	CA	VAL		41.211 -28				3A7
ATOM	1683	СВ	VAL		41.292 -21	3.416 26.60	9 1.00	0.00	3A7
ATOM	1684		1 VAL		41.865 -29	9.803 26.23	7 1.00	0.00	3A7

ATOM	1685	CG2	VAL	253	39.886 -	28.264	25.997		0.00	3A7
ATOM	1686	С	VAL	253	42.532 -	-28.553	28.758		0.00	3A7
ATOM	1687	0	VAL	253	42.684 -		29.404	1.00	0.00	3A7
ATOM	1688	N	LYS	254	43.518 -		28.616	1.00	0.00	3A7
ATOM	1689	CA	LYS	254	44.842 -		29.162	1.00	0.00	3A7 3A7
ATOM	1690	CB	LYS	254	45.735 - 47.220 -		28.706 29.086	1.00	0.00	3A7
ATOM	1691 1692	CG	LYS LYS	254 254	48.143		28.496	1.00	0.00	3A7
MOTA MOTA	1693	CE	LYS	254	48.079		29.199	1.00	0.00	3A7
ATOM	1694	NZ	LYS	254	46.811		28.925	1.00	0.00	3A7
ATOM	1695	c	LYS	254	44.830		30.665	1.00	0.00	3A7
ATOM	1696	o	LYS	254	45.412		31.270	1.00	0.00	3A7
MOTA	1697	N	GLN	255	44.098		31.313	1.00	0.00	3A7
MOTA	1698	CA	GLN	255	43.943		32.753	1.00	0.00	3A7
MOTA	1699	CB	GLN	255	43.122		33.238	1.00	0.00	3A7
MOTA	1700	CG	GLN	255	43.863		33.045	1.00	0.00	3A7
MOTA	1701	CD	GLN	255	42.977		33.535	1.00	0.00 0.00	3A7 3A7
MOTA	1702		GLN	255	43.332 41.801		34.484 32.860	1.00	0.00	3A7
ATOM ATOM	1703 1704	NE2 C	GLN GLN	255 255	43.283		33.282	1.00	0.00	3A7
ATOM	1705	ŏ	GLN	255	43.599		34.372	1.00	0.00	3A7
ATOM	1706	N	ILE	256	42.375		32.490	1.00	0.00	3A7
ATOM	1707	CA	ILE	256	41.679		32.888	1.00	0.00	3A7
ATOM	1708	СВ	ILE	256	40.404	-30.098	32.072	1.00	0.00	3A7
ATOM	1709	CG2	ILE	256	40.068	-31.597	31.831	1.00	0.00	3A7
ATOM	1710	CG1	ILE	256	39.198		32.862	1.00	0.00	3A7
MOTA	1711	CD	ILE	256	39.270		33.277	1.00	0.00	3A7
ATOM	1712	С	ILE	256	42.566		32.826	1.00	0.00	3A7
ATOM	1713	0	ILE	256	42.411		33.627	1.00	0.00 0.00	3A7 3A7
MOTA	1714	N	LYS	257	43.535 44.464		31.881 31.759	1.00	0.00	3A7
ATOM ATOM	1715 1716	CA CB	LYS LYS	257 257		-32.240	30.418	1.00	0.00	3A7
ATOM	1717	CG	LYS	257		-32.548	29.218	1.00	0.00	3A7
MOTA	1718	CD	LYS	257		-32.676	27.864	1.00	0.00	3A7
MOTA	1719	CE	LYS	257		-31.365	27.283	1.00	0.00	3A7
ATOM	1720	NZ	LYS	257		-30.908	27.996	1.00	0.00	3A7
ATOM	1721	С	LYS	257		-32.284	32.873	1.00	0.00	3A7
MOTA	1722	0	LYS	257		-33.343	33.303	1.00	0.00	3A7
ATOM	1723	N	GLU	258		-31.083	33.378	1.00	0.00	3A7 3A7
ATOM	1724	CA	GLU	258		-30.925 -29.519	34.446 34.428	1.00	0.00	3A7
MOTA MOTA	1725 1726	CB CG	GLU	258 258		-29.217	33.141	1.00	0.00	3A7
ATOM	1727	CD	GLU	258		-30.199	33.003	1.00	0.00	3A7
ATOM	1728		GLU	258		-30.202	33.900	1.00	0.00	3A7
ATOM	1729		GLU	258	49.418	-30.958	31.997	1.00	0.00	3A7
ATOM	1730	С	GLU	258		-31.151	35.797	1.00	0.00	3A7
MOTA	1731	0	GLU	258		~31.501	36.763	1.00	0.00	3A7
ATOM	1732	N	GLY	259		-30.971	35.870	1.00	0.00	3A7
ATOM	1733	CA	GLY	259	•	-31.194	37.052 37.051	1.00	0.00 0.00	3A7 3A7
ATOM	1734 1735	c o	GLY GLY	259 259		-32.598 -33.461	36.340	1.00	0.00	3A7
MOTA MOTA	1736	N	ARG	260		-32.842	37.887	1.00	0.00	3A7
ATOM	1737	CA	ARG	260		-34.118	38.133	1.00	0.00	3A7
ATOM	1738	СВ	ARG	260		-34.954	36.853	1.00		3A7
ATOM	1739	CG	ARG	260		-36.233	37.027	1.00		3A7
ATOM	1740	CD	ARG	260		-36.004	37.425	1.00		3A7
MOTA	1741	NE	ARG	260		-35.667	38.882	1.00		3A7
ATOM	1742		ARG	260		-35.260	39.486	1.00		3A7
MOTA	1743		ARG	260		-34.927	40.809	1.00		3A7 3A7
ATOM	1744		ARG	260		-35.174 -34.898	38.781 39.116	1.00		3A7
ATOM ATOM	1745 1746		ARG ARG	260 260		-35.831	38.749	1.00		3A7
ATOM	1747		LEU	261		-34.475	40.403			3A7
ATOM	1748		LEU	261		-34.943	41.438	1.00		3A7
ATOM	1749		LEU	261		-33.853				3A7
ATOM	1750		LEU	261		-32.584	42.630			3A7
ATOM	1751	CD:	LEU	261		-31.737	43.230			3A7
MOTA	1752		LEU	261		-31.708				3A7
ATOM	1753		LEU	261		-35.510				3A7
ATOM	1754		LEU			-36.544 -34.935				3A7 3A7
ATOM	1755		LYS			-34.835 -35.239				3A7
ATOM	1756	CA	LYS	402	40.700	-33.233	77.11/	1.00		J.A.

ATOM	1757	СВ	LYS	262	41.421 -3	34.790	45.462	1.00	0.00	3A7
MOTA	1758	CG	LYS	262	40.810 -3		46.708		0.00	3A7
MOTA	1759	CD	LYS	262	41.515 -3		48.009		0.00	3A7
ATOM	1760	CE	LYS	262	41.066 -		49.233		0.00	3A7
ATOM	1761	NZ	LYS	262	39.611 -		49.468		0.00	3A7
ATOM	1762	C	LYS	262	39.442 -		43.941 43.313		0.00	3A7 3A7
MOTA	1763	0	LYS	262	39.325 -		44.510	1.00	0.00	3A7
ATOM	1764 1765	N CA	GLU	263 263	38.381 -: 37.009 -:		44.438	1.00	0.00	3A7
MOTA MOTA	1766	CB	GLU	263	36.001 -		44.396	1.00	0.00	3A7
ATOM	1767	CG	GLU	263	36.178 -		43.152	1.00	0.00	3A7
ATOM	1768	CD	GLU	263	35.147 -		43.149	1.00	0.00	3A7
ATOM	1769		GLU	263	34.322 -		44.098	1.00	0.00	3A7
ATOM	1770		GLU	263	35.174 -	38.773	42.183	1.00	0.00	3A7
MOTA	1771	С	GLU	263	36.698 -	33.900	45.630	1.00	0.00	3A7
MOTA	1772	0	GLU	263	35.910 -		46.501	1.00	0.00	3A7
ATOM	1773	N	THR	264	37.333 -		45.670	1.00	0.00	3A7
ATOM	1774	CA	THR	264	37.170 -		46.715	1.00	0.00	3A7
ATOM	1775	CB	THR	264	38.280 -		47.757	1.00	0.00	3A7 3A7
ATOM	1776		THR	264	38.329 -		48.352 48.870	1.00	0.00	3A7
ATOM	1777		THR	264 264	38.047 - 37.164 -		46.003	1.00	0.00	3A7
ATOM ATOM	1778 1779	0	THR THR	264	36.480 -		46.415	1.00	0.00	3A7
ATOM	1780	N	GLN	265	37.940 -		44.890	1.00	0.00	3A7
ATOM	1781	CA	GLN	265	38.063 ~		44.052	1.00	0.00	3A7
ATOM	1782	СВ	GLN	265	39.417 -		43.298	1.00	0.00	3A7
ATOM	1783	CG	GLN	265	40.645 -	28.808	44.201	1.00	0.00	3A7
ATOM	1784	CD	GLN	265	40.965 -	30.055	45.032	1.00	0.00	3A7
MOTA	1785	OE1	GLN	265	41.070 -		44.497	1.00	0.00	3A7
MOTA	1786	NE2	GLN	265	41.132 -		46.374	1.00	0.00	3A7
ATOM	1787	С	GLN	265	36.953 -		43.030	1.00	0.00	3A7
MOTA	1788	0	GLN	265	36.287 -		42.802	1.00	0.00	3A7 3A7
ATOM	1789	N	LYS	266	36.738 -		42.404	1.00	0.00 0.00	3A7
ATOM	1790	CA	LYS	266	35.642 - 36.035 -		41.500 40.002	1.00	0.00	3A7
ATOM ATOM	1791 1792	CB CG	LYS LYS	266 266	37.305 -		39.591	1.00	0.00	3A7
ATOM	1793	CD	LYS	266	37.703 -		38.129	1.00	0.00	3A7
ATOM	1794	CE	LYS	266	38.982		37.724	1.00	0.00	3A7
MOTA	1795	NZ	LYS	266	39.346 -		36.320	1.00	0.00	3A7
ATOM	1796	C	LYS	266	35.129 -		41.858	1.00	0.00	3A7
ATOM	1797	0	LYS	266	35.796 -	-32.934	41.655	1.00	0.00	3A7
MOTA	1798	N	HIS	267	33.902 -		42.437	1.00	0.00	3A7
MOTA	1799	CA	HIS	267	33.272		42.940	1.00	0.00	3A7
MOTA	1800		HIS	267	32.504		45.499	1.00	0.00	3A7 3A7
ATOM	1801	CG	HIS	267	31.780		44.815 44.174	1.00	0.00 0.00	3A7
ATOM	1802	CB	HIS	267 267	32.380 · 30.385 ·		45.524	1.00	0.00	3A7
ATOM ATOM	1803 1804		HIS	267	30.489		44.840	1.00	0.00	3A7
ATOM	1805		HIS	267	31.620		45,901	1.00	0.00	3A7
ATOM	1806	c	HIS	267	32.435		41.858	1.00	0.00	3A7
ATOM	1807	ō	HIS	267	32.255	-35.018	41.834	1.00	0.00	3A7
ATOM	1808	N	ARG	268	31.909	-32.963	40.929	1.00	0.00	3A7
MOTA	1809	CA	ARG	268	31.110		39.804	1.00	0.00	3A7
MOTA	1810	CB	ARG	268	29.939		39.501	1.00	0.00	3A7
ATOM	1811	CG	ARG	268	30.357		39.172	1.00	0.00	3A7
ATOM	1812	CD	ARG	268	29.154		38.948	1.00	0.00	3A7 3A7
MOTA	1813	NE	ARG	268	29.664		38.573	1.00	0.00	3A7
ATOM	1814	CZ	ARG	268	28.818 29.328		38.353 37.993	1.00	0.00	3A7
ATOM ATOM	1815 1816		L ARG 2 ARG	268 268	27.470		38.491	1.00	0.00	3A7
ATOM	1817	C	ARG	268	31.997		38.593	1.00	0.00	3A7
ATOM	1818	ŏ	ARG	268	33.012		38.485	1.00	0.00	3A7
ATOM	1819	N	VAL	269	31.604		37.643	1.00	0.00	3A7
ATOM	1820	CA	VAL	269	32.279		36.378	1.00	0.00	3A7
ATOM	1821	СВ	VAL	269	32.595		36.063	1.00	0.00	3A7
MOTA	1822		l VAL		33.733		37.001	1.00	0.00	3A7
MOTA	1823	CG2	VAL		31.340		36.220	1.00	0.00	3A7
MOTA	1824	C	VAL			-33.947	35.315		0.00	3A7
MOTA	1825	0	VAL			-33.712	35.519			3A7
ATOM	1826	N	ASP			-33.642	34.156			3A7 3A7
ATOM	1827	CA	ASP			-32.836	33.096			3A7
ATOM	1828	СВ	ASP	270	31.980	-31.399	33.132	1.00	0.00	JAT

ATOM	1829	CG	ASP	270	33.510 -	-31.368	33.034	1.00	0.00	3A7
ATOM	1830	OD1		270	34.013 -		31.995	1.00	0.00	3A7
ATOM	1831	OD2		270	34.191 -		33.998	1.00	0.00	3A7
MOTA	1832	С	ASP	270	31.710 -		31.781	1.00	0.00	3A7
MOTA	1833	0	ASP	270	32.369 -		31.709	1.00	0.00	3A7
ATOM	1834	N	PHE	271	31.187 -		30.684	1.00	0.00	3A7 3A7
ATOM	1835	CA	PHE	271 271	31.302 - 30.407 -		29.357 28.356	1.00	0.00	3A7
ATOM	1836 1837	CB CG	PHE	271	30.344		27.080	1.00	0.00	3A7
ATOM ATOM	1838	CD1		271	30.012		27.101	1.00	0.00	3A7
ATOM	1839	CD2		271	30.758		25.887	1.00	0.00	3A7
ATOM	1840	CEI		271	30.211		25.972	1.00	0.00	3A7
ATOM	1841	CE2	PHE	271	30.870 -		24.737	1.00	0.00	3A7
ATOM	1842	CZ	PHE	271	30.646	-35.078	24.793	1.00	0.00	3A7
ATOM	1843	C	PHE	271	32.719		28.848	1.00	0.00	3A7
ATOM	1844	0	PHE	271	33.150		28.204	1.00	0.00	3A7
MOTA	1845	N	LEU	272	33.494		29.146	1.00	0.00	3A7
ATOM	1846	CA	LEU	272	34.866		28.716	1.00	0.00	3A7
ATOM	1847	CB	LEU	272	35.455		29.100	1.00	0.00	3A7 3A7
ATOM	1848	CG	LEU	272 272	36.816 · 36.864 ·		28.482 28.078	1.00	0.00	3A7
ATOM ATOM	1849 1850		LEU	272	38.027		29.363	1.00	0.00	3A7
ATOM	1851	C	LEU	272	35.735		29.311	1.00	0.00	3A7
ATOM	1852	ō	LEU	272	36.573		28.634	1.00	0.00	3A7
ATOM	1853	N	GLN	273	35.522		30.606	1.00	0.00	3A7
MOTA	1854	CA	GLN	273	36.255	-34.750	31.288	1.00	0.00	3A7
MOTA	1855	CB	GLN	273	35.890	-34.805	32.788	1.00	0.00	3A7
MOTA	1856	CG	GLN	273	36.853		33.658	1.00	0.00	3A7
MOTA	1857	CD	GLN	273	38.222		33.686	1.00	0.00	3A7
ATOM	1858		GLN	273	38.361		34.234	1.00	0.00	3A7
ATOM	1859		GLN	273	39.247 35.971		33.079 30.668	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	1860 1861	C O	GLN GLN	273 273	36.882		30.456	1.00	0.00	3A7
ATOM	1862	N	LEU	274	34.685		30.310	1.00	0.00	3A7
ATOM	1863	CA	LEU	274		-37.560	29.669	1.00	0.00	3A7
ATOM	1864	СВ	LEU	274	32.718		29.471	1.00	0.00	3A7
ATOM	1865	CG	LEU	274	31.891	-37.798	30.761	1.00	0.00	3A7
ATOM	1866	CD1	LEU	274	30.398	-37.811	30.394	1.00	0.00	3A7
MOTA	1867		LEU	274		-39.060	31.558	1.00	0.00	3A7
MOTA	1868	C	LEU	274		-37.729	28.302	1.00	0.00	3A7
ATOM	1869	0	LEU	274		-38.832	27.930	1.00	0.00	3A7 3A7
ATOM ATOM	1870 1871	N CA	MET MET	275 275		-36.636 -36.702	27.521 26.211	1.00	0.00 0.00	3A7 3A7
ATOM	1872	CB	MET	275		-35.428	25.399	1.00	0.00	3A7
ATOM	1873	CG	MET	275		-35.154	24.962	1.00	0.00	3A7
ATOM	1874	SD	MET	275		-33.829	23.713	1.00	0.00	3A7
ATOM	1875	CE	MET	275	34.315	-32.435	24.786	1.00	0.00	3A7
MOTA	1876	С	MET	275	37.090	-36.951	26.286	1.00	0.00	3A7
ATOM	1877	Ó	MET	275		-37.666	25.458	1.00	0.00	. 3A7
ATOM	1878	N	ILE	276		-36.381	27.305	1.00	0.00	3A7 3A7
ATOM	1879 1880	CA	ILE	276		-36.516	27.488	1.00	0.00	3A7
ATOM ATOM	1881	CB	ILE	276 276		-35.567 -35.906	28.575 29.105	1.00	0.00	3A7
ATOM	1882		ILE	276		-34.100	28.081	1.00	0.00	3A7
MOTA	1883	CD	ILE	276		-33.779	27.011	1.00	0.00	3A7
ATOM	1884	C	ILE	276		-37.926	27.833	1.00	0.00	3A7
MOTA	1885	0	ILE	276		-38.375	27.476	1.00	0.00	3A7
MOTA	1886	И	ASP	277		-38.659	28.548	1.00	0.00	3A7
ATOM	1887	CA	ASP	277		-39.958	29.016	1.00	0.00	3A7
ATOM	1888	СВ	ASP	277		-40.156	30.516	1.00	0.00	3A7
ATOM	1889	CG	ASP	277		-39.210	31.302	1.00	0.00	3A7
ATOM	1890 1891		ASP	277 277		-39.021 -38.657	30.882 32.329	1.00	0.00	3A7 3A7
ATOM ATOM	1891	C	ASP ASP	277		-41.070	28.476		0.00	3A7
ATOM	1893	Ö	ASP	277		-42.095	28.164	1.00	0.00	3A7
ATOM	1894	N	SER			-41.031	28.602	1.00	0.00	3A7
ATOM	1895	CA	SER			-42.176	29.071	1.00	0.00	3A7
MOTA	1896	СВ	SER			-41.818	29.196		0.00	3A7
ATOM	1897	OG	SER			-41.424	27.961		0.00	3A7
MOTA	1898	С	SER			-43.499	28.318			3A7
MOTA	1899	0	SER			-43.792	27.399		0.00	3A7
MOTA	1900	N	GLN	279	37.341	-44.307	28.750	1.00	0.00	3A7

MOTA	1901	CA	GLN	279	37.851 -	45.539	28.167	1.00	0.00	3A7
ATOM	1902	СВ	GLN	279	36.793 -		27.561	1.00	0.00	3A7
ATOM	1903	CG	GLN	279	35.768	47.000	28.593	1.00	0.00	3A7
ATOM	1904	CD	GLN	279	34.775 -	47.928	27.887	1.00	0.00	3A7
ATOM	1905	OE1	GLN	279	35.143 -	49.016	27.428	1.00	0.00	3A7
ATOM	1906	NE2	GLN	279	33.487 -	47.472	27.805	1.00	0.00	3A7
ATOM	1907	С	GLN	279	38.889 -		27.116	1.00	0.00	3A7
ATOM	1908	0	GLN	279	38.687 -	45.481	25.937	1.00	0.00	3A7
ATOM	1909	N	ASN	280	40.027 -	44.587	27.552	1.00	0.00	3A7
ATOM	1910	CA	ASN	280	41.202 -	44.166	26.787	1.00	0.00	3A7
ATOM	1911	CB	ASN	280	42.008 -	45.358	26.209	1.00	0.00	3A7
ATOM	1912	CG	ASN	280	42.430 -	46.296	27.347	1.00	0.00	3A7
ATOM	1913	OD1	ASN	280	41.937 -	47.427	27.447	1.00	0.00	3A7
MOTA	1914	ND2	ASN	280	43.366 -	45.803	28.213	1.00	0.00	3A7
MOTA	1915	С	ASN	280	40.890 -	43.183	25.664	1.00	0.00	3A7
MOTA	1916	0	ASN	280	40.934 -	43.532	24.487	1.00	0.00	3A7
ATOM	1917	N	SER	281	40.551 -	41.923	26.053	1.00	0.00	3A7
MOTA	1918	CA	SER	281	40.076 -	40.803	25.252	1.00	0.00	3A7
ATOM	1919	СВ	SER	281	40.924 -	40.513	23.986	1.00	0.00	3A7
ATOM	1920	OG	SER	281	42.283 -		24.340	1.00	0.00	3A7
ATOM	1921	С	SER	281	38.621 -		24.837	1.00	0.00	3A7
MOTA	1922	0	SER	281	38.131 -		24.021	1.00	0.00	3A7
MOTA	1923	N	LYS	282	37.924 -		25.342	1.00	0.00	3A7
MOTA	1924	CA	LYS	282	36.818 -		24.707	1.00	0.00	3A7
MOTA	1925	СВ	LYS	282	35.459 -		24.620	1.00	0.00	3A7
MOTA	1926	CG	LYS	282	34.288 -		24.294	1.00	0.00	3A7
ATOM	1927	CD	LYS	282	32.914 -		24.590	1.00	0.00	3A7
ATOM	1928	CE	LYS	282	31.744 -		24.357	1.00	0.00	3A7
ATOM	1929	NZ	LYS	282	31.691 -		22.946	1.00	0.00	3A7
MOTA	1930	С	LYS	282	37.194 -		23.334	1.00	0.00	3A7
ATOM	1931	0	LYS	282	37.082 -		22.364	1.00	0.00	3A7
MOTA	1932	N	ASP	283	37.706 -		23.270	1.00	0.00	3A7
MOTA	1933	CA	ASP	283	38.125 -		22.041	1.00	0.00	3A7
ATOM	1934	CB	ASP	283	39.663 -		21.918	1.00	0.00	3A7 3A7
ATOM	1935	CG	ASP	283	40.442 -		22.880	1.00	0.00	3A7
ATOM	1936		ASP	283	41.683 -		22.672	1.00	0.00	3A7
MOTA	1937		ASP	283	39.853 -		23.810 21.948	1.00	0.00	3A7
ATOM	1938 1939	С О	ASP ASP	283 283	37.352 - 37.675 -		22.581	1.00	0.00	3A7
ATOM ATOM	1940	N	SER	284	36.258 -		21.157	1.00	0.00	3A7
ATOM	1941	CA	SER	284	35.513 -		20.782	1.00	0.00	3A7
ATOM	1942	СВ	SER	284	34.115 -		20.210	1.00	0.00	3A7
ATOM	1943	OG	SER	284	34.183 -		19.212	1.00	0.00	3A7
ATOM	1944	c	SER	284	36.266 -		19.834	1.00	0.00	3A7
ATOM	1945	ŏ	SER	284	36.990 -		20.242	1.00	0.00	3A7
ATOM	1946	N	GLU	285	36.113 -		18.521	1.00	0.00	3A7
ATOM	1947	CA	GLU	285	36.639 -		17.634	1.00	0.00	3A7
ATOM	1948	СВ	GLU	285	35.795 -		16.369	1.00	0.00	3A7
MOTA	1949	CG	GLU	285	35.628 -	-47.895	15.591	1.00	0.00	3A7
ATOM	1950	CD	GLU	285	34.752 -	-48.143	14.367	1.00	0.00	3A7
ATOM	1951	OE1	GLU	285	33.566 -	-48.527	14.555	1.00	0.00	3A7
ATOM	1952	OE2	GLU	285	35.255 -	-47.948	13.228	1.00	0.00	3A7
ATOM	1953	С	GLU	285	38.083 -	-48.834	17.309	1.00	0.00	3A7
MOTA	1954	0	GLU	285	38.621 -	-49.477	16.447	1.00	0.00	3A7
MOTA	1955	N	THR	286	38.744		18.009	1.00	0.00	3A7
MOTA	1956	CA	THR	286	40.099		17.894	1.00	0.00	3A7
MOTA	1957	СВ	THR	286	41.251		17.728	1.00	0.00	3A7
MOTA	1958		THR	286	41.071		18.620	1.00	0.00	3A7
ATOM	1959		THR	286	42.623		18.038	1.00	0.00	3A7
ATOM	1960	С	THR	286	40.161		16.868	1.00	0.00	3A7
ATOM	1961	0	THR	286	41.095		16.847	1.00	0.00	3A7
ATOM	1962	N	HIS	287	39.201		15.904	1.00	0.00	3A7
ATOM	1963	CA	HIS	287	39.294		14.676	1.00	0.00	3A7
ATOM	1964		HIS	287	37.806		11.739	1.00	0.00	3A7
MOTA	1965	CG	HIS	287	38.588		12.192	1.00	0.00	3A7
MOTA	1966	CB	HIS	287	38.440		13.541	1.00	0.00	3A7 3A7
ATOM	1967		HIS	287	39.260		10.120	1.00	0.00	3A7
ATOM	1968		HIS	287	39.470		11.189 10.497	1.00	0.00	3A7
MOTA	1969		HIS	287 287	38.251 38.868		14.911	1.00	0.00	3A7
ATOM	1970	C	HIS	287 287	38.868		14.911	1.00	0.00	3A7
MOTA	1971	0	HIS	287 288	39.880		15.122		0.00	3A7
MOTA	1972	N	LYS	288	39.000	-43.223	13.164	1.00	0.00	JAI

ATOM	1973	CA	LYS	288	39.776 -	41.800	15.358	1.00	0.00	3A7
ATOM	1974	СВ	LYS	288	38.889 -		14.340	1.00	0.00	3A7
ATOM	1975	CG	LYS	288	39.415 -		12'. 901	1.00	0.00	3A7
ATOM	1976	CD	LYS	288	38.528 -		11.877	1.00	0.00	3A7
ATOM	1977	CE	LYS	288	39.036 -		10.434	1.00	0.00	3A7
		NZ		288	40.358 -		10.282	1.00	0.00	3A7
ATOM	1978		LYS		39.309		16.767	1.00	0.00	3A7
ATOM	1979	C	LYS	288				1.00	0.00	3A7
MOTA	1980	0	LYS	288	38.116 -		17.030			
ATOM	1981	N	ALA	289	40.290		17.701	1.00	0.00	3A7
MOTA	1982	CA	ALA	289	40.092		19.070	1.00	0.00	3A7
MOTA	1983	СВ	ALA	289	41.158		20.027	1.00	0.00	3A7
MOTA	1984	С	ALA	289	40.164		19.078	1.00	0.00	3A7
MOTA	1985	0	ALA	289	40.670		18.128	1.00	0.00	3A7
ATOM	1986	N	LEU	290	39.624 ·		20.137	1.00	0.00	3A7
MOTA	1987	CA	LEU	290	39.349	-37.401	20.081	1.00	0.00	3A7
ATOM	1988	CB	LEU	290	38.229	-37.004	21.014	1.00	0.00	3A7
MOTA	1989	CG	LEU	290	36.888	-37.703	20.701	1.00	0.00	3A7
ATOM	1990	CD1	LEU	290	35.892	-37.512	21.861	1.00	0.00	3A7
ATOM	1991		LEU	290	36.312	-37.221	19.355	1.00	0.00	3A7
ATOM	1992	C	LEU	290	40.550		20.350	1.00	0.00	3A7
ATOM	1993	ō	LEU	290	41.191		21.390	1.00	0.00	3A7
ATOM	1994	N	SER	291	40.854		19.352	1.00	0.00	3A7
ATOM	1995	CA	SER	291	41.954		19.363	1.00	0.00	3A7
					42.455		17.928	1.00	0.00	3A7
ATOM	1996	CB	SER	291	41.422		17.030	1.00	0.00	3A7
MOTA	1997	OG	SER	291						
ATOM	1998	С	SER	291	41.471		19.957	1.00	0.00	3A7
MOTA	1999	O	SER	291	40.275		19.991	1.00	0.00	3A7
MOTA	2000	N	ASP	292	42.400		20.410	1.00	0.00	3A7
MOTA	2001	CA	ASP	292	42.071		21.064	1.00	0.00	3A7
ATOM	2002	СВ	ASP	292	43.338		21.556	1.00	0.00	3A7
MOTA	2003	CG	ASP	292	44.042		22.570	1.00	0.00	3A7
MOTA	2004	OD1	ASP	292	43.426		23.629	1.00	0.00	3A7
MOTA	2005	OD2	ASP	292	45.204	-32.050	22.298	1.00	0.00	3A7
MOTA	2006	С	ASP	292	41.334	-30.471	20.170	1.00	0.00	3A7
ATOM	2007	0	ASP	292	40.568	-29.641	20.643	1.00	0.00	3A7
MOTA	2008	N	LEU	293	41.506	-30.616	18.834	1.00	0.00	3A7
ATOM	2009	CA	LEU	293	40.836	-29.795	17.858	1.00	0.00	3A7
ATOM	2010	СВ	LEU	293	41.527	-29.876	16.490	1.00	0.00	3A7
ATOM	2011	CG	LEU	293		-29.436	16.506	1.00	0.00	3A7
ATOM	2012		LEU	293		-29.663	15.129	1.00	0.00	3A7
ATOM	2013		LEU	293		-27.976	16.965	1.00	0.00	3A7
ATOM	2014	c	LEU	293		-30.187	17.711	1.00	0.00	3A7
ATOM	2015	ŏ	LEU	293		-29.340	17.738	1.00	0.00	3A7
ATOM	2016	N	GLU	294		-31.502	17.619	1.00	0.00	3A7
	2017	CA	GLU	294		-31.998	17.504	1.00	0.00	3A7
MOTA			GLU	294		-33.523	17.310	1.00	0.00	3A7
ATOM	2018	CB						1.00	0.00	3A7
MOTA	2019	CG	GLU	294		-33.957	15.942		0.00	3A7
MOTA	2020	CD	GLU	294		-35.480	15.850	1.00		
ATOM	2021	OE1		294	•	-36.040	15.905	1.00	0.00	3A7
MOTA	2022	OE2		294		-36.104	15.722	1.00	0.00	3A7
MOTA	2023	С	GLU	294		-31.676	18.723	1.00	0.00	3A7
MOTA	2024	0	GLU	294	35.776	-31.192	18.632	1.00	0.00	3A7
ATOM	2025	N	LEU	295		-31.876	19.909	1.00	0.00	3A7
MOTA	2026	CA	LEU	295		-31.573	21.190	1.00	0.00	3A7
MOTA	2027	CB	LEU	295		-31.878	22.313	1.00	0.00	3A7
MOTA	2028	CG	LEU	295	38.311	-33.358	22.435	1.00	0.00	3A7
ATOM	2029	CD1	LEU	295	39.434	-33.555	23.470	1.00	0.00	3A7
MOTA	2030	CD2	LEU	295	37.094	-34.206	22.783	1.00	0.00	3A7
ATOM	2031	С	LEU	295	36.535	-30.119	21.312	1.00	0.00	3A7
ATOM	2032	0	LEU	295	35.404	-29.765	21.643	1.00	0.00	3A7
MOTA	2033	N	MET	296		-29.212	21.017	1.00	0.00	3A7
ATOM	2034	CA	MET	296		-27.783	21.050	1.00		3A7
MOTA	2035	СB	MET	296		-27.070	20.647	1.00		3A7
ATOM	2036	CG	MET	296		-25.578	20.350	1.00		3A7
ATOM	2030	SD	MET	296		-24.717	20.404	1.00		3A7
				296		-25.540	18.974	1.00		3A7
ATOM	2038	CE	MET			-23.340		1.00		3A7
ATOM	2039	C	MET	296						3A7 3A7
ATOM	2040	0	MET	296		-26.566		1.00		3A7 3A7
ATOM	2041	N	ALA	297		-27.882	18.877	1.00		
ATOM	2042	CA	ALA	297		-27.555		1.00		3A7
MOTA	2043	СВ	ALA			-28.182		1.00		3A7
MOTA	2044	C	ALA	297	33.783	-27.978	18.300	1.00	0.00	3A7

ATOM	2045	0	ALA	297	32.817 -	-27.301	17.986	1.00	0.00	3A7
ATOM	2046	N	GLN	298	33.648		19.085	1.00	0.00	3A7
ATOM	2047	CA	GLN	298	32.385		19.640	1.00	0.00	3A7
ATOM	2048	СВ	GLN	298	32.482		20.248	1.00	0.00	3A7
ATOM	2049	CG	GLN	298	32.651		19.207	1.00	0.00	3A7
ATOM	2050	CD	GLN	298	32.958		19.922	1.00	0.00	3A7
		OE1		298	34.080		20.400	1.00	0.00	3A7
ATOM	2051		GLN		31.939		19.977	1.00	0.00	3A7
ATOM	2052	NE2		298			20.719	1.00	0.00	3A7
MOTA	2053	c	GLN	298	31.922					
MOTA	2054	0	GLN	298	30.773		20.728	1.00	0.00	3A7
ATOM	2055	N	SER	299	32.831		21.630	1.00	0.00	3A7
MOTA	2056	CA	SER	299	32.535		22.690	1.00	0.00	3A7
MOTA	2057	CB	SER	299	33.759		23.597	1.00	0.00	3A7
ATOM	2058	OG	SER	299	34.175		24.141	1.00	0.00	3A7
MOTA	2059	С	SER	299	32.097		22.158	1.00	0.00	3A7
MOTA	2060	0	SER	299	31.185		22.698	1.00	0.00	3A7
ATOM	2061	N	ILE	300	32.719		21.047	1.00	0.00.	3A7
ATOM	2062	CA	ILE	300	32.361	-24.170	20.361	1.00	0.00	3A7
MOTA	2063	СВ	ILE	300	33.321	-23.832	19.229	1.00	0.00	3a7
ATOM	2064	CG2	ILE	300	32.843	-22.603	18.412	1.00	0.00	3A7
MOTA	2065	CG1	ILE	300	34.732	-23.560	19.774	1.00	0.00	3A7
ATOM	2066	CD	ILE	300	35.811	-23.539	18.691	1.00	0.00	3A7
ATOM	2067	С	ILE	300	30.987	-24.293	19.764	1.00	0.00	3A7
ATOM	2068	Ó	ILE	300	30.162		19.914	1.00	0.00	3A7
ATOM	2069	N	ILE	301	30.695		19.092	1.00	0.00	3A7
ATOM	2070	CA	ILE	301	29.418		18.455	1.00	0.00	3A7
ATOM	2071	СВ	ILE	301	29.475		17.553	1.00	0.00	3A7
ATOM	2072		ILE	301	28.192		17.525	1.00	0.00	3A7
ATOM	2073		ILE	301	29.774		16.091	1.00	0.00	3A7
ATOM	2074	CD	ILE	301	31.053		15.869	1.00	0.00	3A7
ATOM	2075	c	ILE	301	28.303		19.465	1.00	0.00	3A7
				301	27.182		19.205	1.00	0.00	3A7
ATOM	2076	0	ILE		28.584		20.673	1.00	0.00	3A7
ATOM	2077	N	PHE	302						
ATOM	2078	CA	PHE	302		-26.507	21.709	1.00	0.00	3A7
MOTA	2079	CB	PHE	302		-27.306	22.878	1.00	0.00	3A7
MOTA	2080	CG	PHE	302		-28.790	22.660	1.00	0.00	3A7
ATOM	2081		PHE	302		-29.335	21.379	1.00	0.00	3A7
ATOM	2082		PHE	302		-29.577	23.757	1.00	0.00	3A7
MOTA	2083		PHE	302		-30.584	21.188	1.00	0.00	3A7
MOTA	2084	CE2		302		-30.829	23.567	1.00	0.00	3A7
MOTA	2085	CZ	PHE	302		-31.311	22.282	1.00	0.00	3A7
ATOM	2086	С	PHE	302		-25.150	22.252	1.00	0.00	3A7
ATOM	2087	0	PHE	302		-24.892	22.478	1.00	0.00	3A7
MOTA	2088	N	ILE	303	28.134	-24.221	22.452	1.00	0.00	3A7
MOTA	2089	CA	ILE	303	27.866	-22.889	22.966	1.00	0.00	3A7
MOTA	2090	СВ	ILE	303	29.091	-22.188	23.539	1.00	0.00	3A7
ATOM	2091	CG2	ILE	303	28.716	-20.768	24.038	1.00	0.00	3A7
ATOM	2092	CG1	ILE	303	29.642	-23.043	24.700	1.00	0.00	3A7
ATOM	2093	CD	ILE	303	30.952	-22.513	25.280	1.00	0.00	3A7
ATOM	2094	С	ILE	303	27.215	-22.030	21.914	1.00	0.00	3A7
ATOM	2095	0	ILE	303		-21.376	22.173	1.00	0.00	3A7
ATOM	2096	N	PHE	304	27.728	-22.042	20.671	1.00	0.00	3A7
ATOM	2097	CA	PHE	304		-21.301	19.548	1.00	0.00	3A7
ATOM	2098	СВ	PHE	304		-21.579	18.314	1.00	0.00	3A7
ATOM	2099	CG	PHE	304		-20.996	16.996	1.00	0.00	3A7
ATOM	2100		PHE	304		-19.644	16.704	1.00	0.00	3A7
ATOM	2101		PHE	304		-21.829	16.036	1.00	0.00	3A7
ATOM	2102		PHE	304		-19.134	15.472	1.00	0.00	3A7
ATOM	2103		PHE	304		-21.320	14.811	1.00	0.00	3A7
ATOM	2104	CZ	PHE	304		-19.970	14.526	1.00	0.00	3A7
	2105		PHE			-21.649	19.207	1.00	0.00	3A7
MOTA MOTA	2105	C O	PHE	304 304		-20.780	19.129	1.00	0.00	3A7
	2107	N				-22.954	19.027	1.00	0.00	3A7
ATOM			ALA	305 305		-23.428	18.672	1.00	0.00	3A7
MOTA	2108	CA	ALA	305						
ATOM	2109	CB	ALA	305		-24.883	18.216	1.00	0.00	3A7
ATOM	2110	C	ALA	305		-23.354	19.820	1.00	0.00	3A7
ATOM	2111	0	ALA	305		-23.132	19.620	1.00	0.00	3A7
ATOM	2112	N	GLY	306		-23.533	21.051	1.00	0.00	3A7
ATOM	2113	CA	GLY	306		-23.642	22.219	1.00	0.00	3A7
ATOM	2114	С	GLY	306		-22.346	22.888	1.00	0.00	3A7
MOTA	2115	0	GLY	306		-22.258	23.561	1.00	0.00	3A7
MOTA	2116	N	TYR	307	23.359	-21.285	22.742	1.00	0.00	3A7

ATOM	2117	CA	TYR	307	23.134 -20.054	23.474	1.00	0.00	3A7
ATOM	2118	СВ	TYR	307	24.473 -19.279	23.690	1.00	0.00	3A7
ATOM	2119	CG	TYR	307	24.492 -17.764		1.00	0.00	3A7
MOTA	2120	CD1		307	23.675 -16.927		1.00	0.00	3A7
MOTA	2121	CD2		307	25.364 -17.182		1.00	0.00	3A7
ATOM	2122	CE1		307	23.720 -15.545		1.00	0.00	3A7 3A7
ATOM	2123	CE2		307 307	25.420 -15.801 24.595 -14.980		1.00	0.00	3A7
ATOM ATOM	2124 2125	CZ OH	TYR TYR	307	24.653 -13.578		1.00	0.00	3A7
ATOM	2126	C	TYR	307	22.056 -19.224		1.00	0.00	3A7
ATOM	2127	ŏ	TYR	307	21.092 -18.851		1.00	0.00	3A7
ATOM	2128	N	GLU	308	22.222 -18.888		1.00	0.00	3A7
ATOM	2129	CA	GLU	308	21.442 -17.887	20.875	1.00	0.00	3A7
ATOM	2130	CB	GLU	308	22.048 -17.593	19.488	1.00	0.00	3A7
MOTA	2131	CG	GLU	308	22.280 -18.86		1.00	0.00	3A7
ATOM	2132	CD	GLU	308	23.057 -18.569		1.00	0.00	3A7
ATOM	2133		GLU	308	23.277 -17.372		1.00	0.00	3A7
ATOM	2134		GLU	308	23.430 -19.55		1.00	0.00	3A7 3A7
ATOM	2135	C	GLU	308 308	20.007 -18.253 19.119 -17.42		1.00	0.00	3A7
ATOM	2136 2137	O N	GLU THR	309	19.741 -19.53		1.00	0.00	3A7
ATOM ATOM	2138	CA	THR	309	18.413 -20.05		1.00	0.00	3A7
MOTA	2139	CB	THR	309	18.504 -21.43		1.00	0.00	3A7
ATOM	2140		THR	309	17.244 -21.87		1.00	0.00	3A7
ATOM	2141		THR	309	19.256 -22.43		1.00	0.00	3A7
ATOM	2142	С	THR	309	17.592 -20.08	21.350	1.00	0.00	3A7
ATOM	2143	0	THR	309	16.436 -19.68		1.00	0.00	3A7
MOTA	2144	N	THR	310	18.187 -20.51		1.00	0.00	3A7
MOTA	2145	CA	THR	310	17.519 -20.56		1.00	0.00	3A7
ATOM	2146	CB	THR	310	18.271 -21.43		1.00	0.00	3A7
ATOM	2147		THR	310	18.739 -22.60		1.00	0.00	3λ7 3 λ 7
ATOM	2148		THR	310 310	17.383 -21.83 17.233 -19.20		1.00	0.00	3A7
ATOM ATOM	2149 2150	C O	THR THR	310	16.168 -18.98		1.00	0.00	3A7
ATOM	2151	N	SER	311	18.147 -18.22		1.00	0.00	3A7
MOTA	2152	CA	SER	311	17.925 -16.88		1.00	0.00	3A7
ATOM	2153	СВ	SER	311	19.171 -15.99		1.00	0.00	3A7
ATOM	2154	OG	SER	311	20.346 -16.71	0 24.906	1.00	0.00	3A7
ATOM	2155	С	SER	311	16.857 -16.19		1.00	0.00	3A7
ATOM	2156	0	SER	311	15.998 -15.51		1.00	0.00	3A7
MOTA	2157	N	SER	312	16.848 -16.36		1.00	0.00	3A7
ATOM	2158	CA	SER	312	15.858 -15.76		1.00	0.00	3A7 3A7
ATOM	2159 2160	CB OG	SER SER	312 312	16.203 -15.89 16.398 -17.24		1.00	0.00	3A7
ATOM ATOM	2161	C	SER	312	14.473 -16.33		1.00	0.00	3A7
ATOM	2162	ŏ	SER	312	13.477 -15.64		1.00	0.00	3A7
ATOM	2163	N	VAL	313	14.376 -17.60		1.00	0.00	3A7
ATOM	2164	CA	VAL	313	13.115 -18.23		1.00	0.00	3A7
ATOM	2165	ÇВ	VAL	313	13.262 -19.73		1.00	0.00	. 3A7
MOTA	2166		VAL	313	12.003 -20.44		1.00	0.00	3A7
ATOM	2167		VAL	313	13.426 -20.12		1.00	0.00	3A7
MOTA	2168	С	VAL	313	12.555 -17.71	2 23.971	1.00	0.00	3A7 3A7
MOTA	2169	0	VAL	313	11.368 -17.42 13.406 -17.52		1.00	0.00	3A7
MOTA MOTA	2170 2171	N CA	LEU LEU	314 314	13.003 -16.99			0.00	3A7
MOTA	2172	СВ	LEU	314	14.178 -17.03			0.00	3A7
ATOM	2173	CG	LEU	314	14.712 -18.44			0.00	3A7
ATOM	2174		LEU	314	16.160 -18.40			0.00	3A7
ATOM	2175		LEU	314	13.817 -19.18			0.00	3A7
ATOM	2176	С	LEU	314	12.519 -15.57		1.00	0.00	3A7
MOTA	2177	0	LEU	314	11.490 -15.20			0.00	3A7
ATOM	2178	N	SER	315	13.252 -14.74			0.00	3A7
ATOM	2179	CA	SER	315	12.914 -13.35			0.00	3A7
ATOM	2180	CB	SER	315	14.033 -12.60			0.00	3A7 3A7
ATOM	2181	OG	SER	315 315	15.234 -12.63 11.625 -13.20				3A7
ATOM ATOM	2182 2183	С 0	SER SER	315	10.814 -12.3				3A7
ATOM	2184	N	PHE	316	11.391 -14.0				3A7
ATOM	2185	CA	PHE	316	10.164 -14.0				3A7
ATOM	2186	СВ	PHE	316	10.264 -14.9				3A7
ATOM	2187	CG	PHE	316	10.697 -14.0				3A7
ATOM	2188		I PHE		11.810 -14.4	39 19.342	1.00	0.00	3A7

ATOM	2189	CD2	PHE	316 -	9.933 -	-12.985	19.709	1.00	0.00	3A7
ATOM	2190	CEl	PHE	316	12.165 -	-13.699	18.217	1.00	0.00	3A7
MOTA	2191	CE2	PHE	316	10.281 -	-12.246	18.582	1.00	0.00	3A7
MOTA	2192	CZ	PHE	316	11.402 -		17.837	1.00	0.00	3A7
ATOM	2193	С	PHE	316	9.015		23.406	1.00	0.00	3A7
MOTA	2194	0	PHE	316	7.891		23.296	1.00	0.00	3A7
MOTA	2195	N	ILE	317	9.257		24.306	1.00	0.00	3A7
ATOM	2196	CA	ILE	317	8.200		25.144	1.00	0.00	3A7
ATOM	2197	CB	ILE	317	8.522		26.022	1.00	0.00	3A7 3A7
ATOM	2198 2199	CG2 CG1		317 317	7.716	-17.434 -18.749	27.357 25.331	1.00	0.00	3A7
ATOM ATOM	2200	CD	ILE	317		-19.340	24.419	1.00	0.00	3A7
ATOM	2201	C	ILE	317		-15.117	26.091	1.00	0.00	3A7
ATOM	2202	ō	ILE	317		-14.997	26.274	1.00	0.00	3A7
ATOM	2203	N	ILE	318		-14.313	26.715	1.00	0.00	3A7
MOTA	2204	CA	ILE	318	8.192	-13.252	27.635	1.00	0.00	3A7
MOTA	2205	CB	ILE	318	9.425	-12.624	28.274	1.00	0.00	3A7
MOTA	2206	CG2	ILE	318		-11.357	29.092	1.00	0.00	3A7
ATOM	2207	CG1		318	10.087		29.181	1.00	0.00	3A7
MOTA	2208	CD	ILE	318	11.481		29.665	1.00	0.00	3A7
ATOM	2209	C	ILE	318		-12.213	26.942	1.00	0.00	3A7
ATOM	2210	0	ILE	318		-11.802	27.441	1.00	0.00 0.00	3A7 3A7
ATOM	2211 2212	N	TYR	319 319		-11.823 -10.893	25.716 24.906	1.00	0.00	3A7
ATOM ATOM	2212	CA CB	TYR TYR	319		-10.658	23.571	1.00	0.00	3A7
ATOM	2214	CG	TYR	319	6.940	-9.879	22.557	1.00	0.00	3A7
ATOM	2215		TYR	319	6.414	-8.628	22.863	1.00	0.00	3A7
ATOM	2216		TYR	319	6.693	-10.438	21.301	1.00	0.00	3A7
MOTA	2217	CE1	TYR	319	5.597	-7.976	21.949	1.00	0.00	3A7
MOTA	2218		TYR	319	5.898	-9.773	20.375	1.00	0.00	3A7
ATOM	2219	CZ	TYR	319	5.336	-8.544	20.704	1.00	0.00	3A7
ATOM	2220	ОН	TYR	319	4.491	-7.887	19.783 24.631	1.00	0.00	3A7 3A7
ATOM ATOM	2221 2222	C O	TYR TYR	319 319		-11.359 -10.588	24.752	1.00	0.00	3A7
ATOM	2223	N	GLU	320		-12.651	24.277	1.00	0.00	3A7
ATOM	2224	CA	GLU	320		-13.205	23.952	1.00	0.00	3A7
ATOM	2225	CB	GLU	320	4.190	-14.545	23.220	1.00	0.00	3A7
ATOM	2226	CG	GLU	320		-14.416	21.829	1.00	0.00	3A7
MOTA	2227	CD	GLU	320		-13.768	20.915	1.00	0.00	3A7
ATOM	2228		GLU	320		-12.634	20.435	1.00	0.00	3A7 3A7
ATOM ATOM	2229 2230	C C	GLU	320 320		-14.384 -13.345	20.681 25.140	1.00	0.00	3A7
ATOM	2231	Ö	GLU	320		-13.087	25.041	1.00	0.00	3A7
ATOM	2232	N	LEU	321		-13.705	26.321	1.00	0.00	3A7
ATOM	2233	CA	LEU	321		-13.799	27.537	1.00	0.00	3A7
ATOM	2234	СB	LEU	321	3.805	-14.427	28.662	1.00	0.00	3A7
MOTA	2235	CG	LEU	321		-15.941	28.472	1.00	0.00	3A7
ATOM	2236		LEU	321		-16.456	29.453	1.00	0.00	3A7
ATOM	.2237		LEU	321		-16.706	28.641	1.00	0.00	3A7 3A7
ATOM ATOM	2238 2239	С 0	LEU LEU	321 321		-12.447 -12.302	28.007 28.509	1.00	0.00 0.00	3A7
ATOM	2240	N	ALA	322		-11.421		1.00		3A7
ATOM	2241	CA	ALA	322		-10.068	28.220	1.00	0.00	3A7
ATOM	2242	СВ	ALA	322	4.351	-9.229	28.225	1.00	0.00	3A7
ATOM	2243	С	ALA	322	2.044	-9.469	27.279	1.00	0.00	3A7
ATOM	2244	0	ALA	322	1.166	-8.702	27.668	1.00	0.00	3A7
ATOM	2245	N	THR		2.110	-9.863	25.996	1.00	0.00	3A7
MOTA	2246	CA	THR		1.174 1.714	-9.402	25.006 23.612	1.00	0.00	3A7 3A7
ATOM . ATOM	2247 2248	CB	THR THR			-9.509 -10.786	23.012	1.00		3A7
ATOM	2249		THR		2.782	-8.417	23.418	1.00		3A7
ATOM	2250	c	THR			-10.105	25.063	1.00		3A7
ATOM	2251	ō	THR		-1.132	-9.627	24.486	1.00		3A7
MOTA	2252	N	HIS	324		-11.241	25.774	1.00		3A7
MOTA	2253	CA	HIS			-12.018	25.882	1.00		3A7
ATOM	2254		HIS			-12.554	22.767	1.00		3A7
ATOM	2255	CG	HIS			-13.139 -13.311	23.576 25.087	1.00		3A7 3A7
ATOM ATOM	2256 2257	CB NE2	HIS HIS			-13.311	21.617	1.00		3A7
ATOM	2258		HIS			-13.016				3A7
ATOM	2259		HIS			-12.187				3A7
ATOM	2260	С	HIS			-12.327		1.00		3A7

ATOM	2261	0	HIS	324	-1.410 -	-13.448	27.764	1.00	0.00	3A7
MOTA	2262	N	PRO	325	-2.246	-11.398	28.139	1.00	0.00	3A7
MOTA	2263	CA	PRO	325	-2.362 -	-11.530	29.587	1.00	0.00	3A7
ATOM	2264	CD	PRO	325	-2.664		27.697	1.00	0.00	3A7
MOTA	2265	CB	PRO	325	-3.005		30.049	1.00	0.00	3A7
ATOM	2266	CG	PRO	325	-2.634	-9.212	28.959	1.00	0.00	3A7
ATOM	2267	C	PRO	325	-3.219		30.001	1.00	0.00 0.00	3A7 3A7
ATOM	2268	0	PRO	325 326	-2.994 ·		31.072 29.162	1.00	0.00	3A7
ATOM ATOM	2269 2270	N CA	ASP ASP	326	-5.016		29.448	1.00	0.00	3A7
ATOM	2271	СВ	ASP	326	-6.108		28.372	1.00	0.00	3A7
ATOM	2272	CG	ASP	326	-7.091		28.363	1.00	0.00	3A7
ATOM	2273		ASP	326	-7.016		29.271	1.00	0.00	3A7
ATOM	2274		ASP	326	-7.946		27.437	1.00	0.00	3A7
ATOM	2275	С	ASP	326	-4.191	-15.557	29.518	1.00	0.00	3A7
ATOM	2276	0	ASP	326	-4.391	-16.408	30.379	1.00	0.00	3A7
ATOM	2277	N	VAL	327	-3.192		28.617	1.00	0.00	3A7
MOTA	2278	CA	VAL	327	-2.308		28.551	1.00	0.00	3A7
ATOM	2279	СВ	VAL	327	-1.522		27.249	1.00	0.00	3A7
ATOM	2280		VAL	327	-0.634		27.189	1.00	0.00	3A7 3A7
ATOM	2281		VAL	327	-2.526		26.078 29.718	1.00	0.00 0.00	3A7
ATOM	2282	C	VAL VAL	327 327	-1.357 -1.126		30.353	1.00	0.00	3A7
ATOM ATOM	2283 2284	O N	GLN	328	-0.822		30.057	1.00	0.00	3A7
ATOM	2285	CA	GLN	328		-15.440	31.190	1.00	0.00	3A7
ATOM	2286	СВ	GLN	328		-13.994	31.280	1.00	0.00	3A7
ATOM	2287	CG	GLN	328		-13.874	31.956	1.00	0.00	3A7
ATOM	2288	CD	GLN	328	2.430	-12.432	31.850	1.00	0.00	3A7
ATOM	2289	OE1	GLN	328		-11.512	31.507	1.00	0.00	3A7
ATOM	2290	NE2	GLN	328		-12.247	32.162	1.00	0.00	3A7
MOTA	2291	C	GLN	328		-15.809	32.500	1.00	0.00	3A7
ATOM	2292	0	GLN	328		-16.448	33.339	1.00	0.00	3A7
ATOM	2293	N	GLN	329		-15.438	32.692	1.00	0.00	3A7 3A7
ATOM	2294	CA	GLN	329		-15.749 -15.032	33.879 33.870	1.00	0.00	3A7
ATOM ATOM	2295 2296	CB CG	GLN GLN	329 329		-13.525	34.148	1.00	0.00	3A7
ATOM	2297	CD	GLN	329		-12.882	34.023	1.00	0.00	3A7
ATOM	2298		GLN	329		-13.175	34.813	1.00	0.00	3A7
ATOM	2299	NE2		329		-11.987	33.000	1.00	0.00	3A7
ATOM	2300	С	GLN	329	-2.821	-17.226	34.022	1.00	0.00	3A7
MOTA	2301	0	GLN	329		-17.780	35.102	1.00	0.00	3A7
ATOM	2302	N	LYS	330		-17.913	32.907	1.00	0.00	3A7
ATOM	2303	CA	LYS	330		-19.343	32.883	1.00	0.00	3A7
ATOM	2304	CB	LYS	330		-19.754	31.503	1.00	0.00	3A7 3A7
ATOM	2305	CG	LYS	330 330		-21.169 -21.428	31.446 30.124	1.00	0.00	3A7
ATOM ATOM	2306 2307	CD	LYS LYS	330		-22.799	30.054	1.00	0.00	3A7
ATOM	2308	NZ	LYS	330		-22.943	31.113	1.00	0.00	3A7
ATOM	2309	c	LYS	330		-20.090	33.241	1.00	0.00	3A7
ATOM	2310	ō	LYS	330		~21.027	34.040	1.00	0.00	3A7
MOTA	2311	N	VAL	331	-0.946	-19.618	32.704	1.00	0.00	3A7
ATOM	2312	CA	VAL	331		-20.189	32.957	1.00	0.00	3A7
ATOM	2313	СВ	VAL	331		-19.605	32.030	1.00	0.00	3A7
ATOM	2314		VAL	331		-20.076	32.382	1.00	0.00	3A7
MOTA	2315		YAL	331		-20.072	30.601 34.390	1.00	0.00	3A7 3A7
ATOM	2316	C	VAL	331		-19.992 -20.919	35.023	1.00	0.00 0.00	3A7
ATOM ATOM	2317 2318	о И	VAL GLN	331 332		-18.783	34.951	1.00	0.00	3A7
ATOM	2319	CA	GLN	332		-18.455	36.319	1.00	0.00	3A7
ATOM	2320	СВ	GLN	332		-16.968	36.628	1.00	0.00	3A7
ATOM	2321	CG	GLN	332		-16.072	36.011	1.00	0.00	3A7
ATOM	2322	CD	GLN	332		-14.601	36.311	1.00		3A7
ATOM	2323		GLN	332		-13.947	37.057	1.00		3A7
ATOM	2324	NEZ	2 GLN	332		-14.079	35.701	1.00		3A7
MOTA	2325	С	GLN	332		-19.234	37.311	1.00		3A7
ATOM	2326	0	GLN			-19.634	38.351	1.00		3A7
ATOM	2327	N	LYS			-19.512	36.991	1.00		3A7 3A7
ATOM	2328	CA	LYS			-20.320				3A7 3A7
ATOM	2329	CB	LYS			-20.312 -21.052				3A7
ATOM ATOM	2330 2331	CD CD	LYS LYS			-20.945				3A7
MOTA	2332	CE	LYS			-21.617				3A7
0.1	2332		2							

ATOM	2333	NZ	LYS	333	-7.518 -2	21.516	35.576	1.00	0.00	3A7
ATOM	2334	С	LYS	333	-1.600 -2		37.882	1.00	0.00	3A7
ATOM	2335	0	LYS	333	~1.547 -2	22.344	38.954	1.00	0.00	3A7
ATOM	2336	N	GLU	334	-1.171 -2	22.295	36.728	1.00	0.00	3A7
MOTA	2337	CA	GLU	334	-0.533 -2	23.579	36.649	1.00	0.00	3A7
ATOM	2338	CB	GLU	334	-0.149 -		35.224	1.00	0.00	3A7
MOTA	2339	CG	GLU	334	-0.038 -		35.122	1.00	0.00	3A7
ATOM	2340	CD	GLU	334	0.087 -		33.672	1.00	0.00	3A7
ATOM	2341	OE1		334	-0.736 -		33.251	1.00	0.00 0.00	3A7 3A7
ATOM	2342		GLU	334	1.007 -: 0.701 -:		32.971 37.472	1.00	0.00	3A7
ATOM	2343 2344	с 0	GLU	334 334	0.701 -		38.236	1.00	0.00	3A7
ATOM ATOM	2344	N	ILE	335	1.627 -		37.370	1.00	0.00	3A7
ATOM	2346	CA	ILE	335	2.874 -		38.098	1.00	0.00	3A7
ATOM	2347	СВ	ILE	335	3.672 -		37.679	1.00	0.00	3A7
ATOM	2348		ILE	335	4.884 -		38.599	1.00	0.00	3A7
ATOM	2349	CG1	ILE	335	4.128 -	21.660	36.215	1.00	0.00	3A7
ATOM	2350	CD	ILE	335	4.634 -	20.360	35.597	1.00	0.00	3A7
ATOM	2351	С	ILE	335	2.643 -	22.684	39.587	1.00	0.00	3A7
MOTA	2352	0	ILE	335	3.219 -		40.320	1.00	0.00	3A7
ATOM	2353	N	ASP	336	1.727 -		40.071	1.00	0.00	3A7
ATOM	2354	CA	ASP	336	1.416 -		41.476	1.00	0.00	3A7
MOTA	2355	CB	ASP	336	0.411 -		41.750	1.00	0.00	3A7 3A7
ATOM	2356	CG	ASP	336	1.021 -		41.420	1.00	0.00	3A7
ATOM	2357		ASP	336	2.243 - 0.255 -		41.123	1.00 1.00	0.00 0.00	3A7
ATOM ATOM	2358 2359	C C	ASP ASP	336 336	0.838 -		42.010	1.00	0.00	3A7
ATOM	2360	0	ASP	336	1.183 -		43.106	1.00	0.00	3A7
ATOM	2361	N	THR	337	-0.022 -		41.213	1.00	0.00	3A7
ATOM	2362	CA	THR	337	-0.701 -		41.571	1.00	0.00	3A7
ATOM	2363	СВ	THR	337	-1.854 -	25.156	40.609	1.00	0.00	3A7
ATOM	2364	OG1	THR	337	-2.791 -	24.092	40.721	1.00	0.00	3A7
ATOM	2365	CG2	THR	337	-2.601 -		40.896	1.00	0.00	3A7
MOTA	2366	С	THR	337	0.216 -		41.595	1.00	0.00	3A7
ATOM	2367	0	THR	337	0.055 -		42.433	1.00	0.00	3A7
ATOM	2368	N	VAL	338	1.202 -		40.667	1.00	0.00	3A7
MOTA	2369	CA	VAL	338	2.055 -		40.503	1.00	0.00	3A7 3A7
MOTA	2370	CB	VAL	338	2.466 - 3.403 -		39.051 38.900	1.00	0.00	3A7
ATOM	2371 2372		VAL VAL	338 338	1.182 -		38.226	1.00	0.00	3A7
ATOM ATOM	2373	C	VAL	338	3.261 -		41.404	1.00	0.00	3A7
ATOM	2374	Ö	VAL	338	3.589 -		42.113	1.00	0.00	3A7
ATOM	2375	N	LEU	339	3.950 -		41.421	1.00	0.00	3 A 7
ATOM	2376	CA	LEU	339	5.053 -		42.331	1.00	0.00	3A7
ATOM	2377	СВ	LEU	339	6.213 -	-25.014	41.736	1.00	0.00	3A7
ATOM	2378	CG	LEU	339	7.082 -	-25.819	40.766	1.00	0.00	3A7
MOTA	2379		LEU	339	8.159		40.176	1.00	0.00	3A7
ATOM	2380		LEU	339	7.715		41.439	1.00	0.00	3A7
ATOM	2381	C	LEU	. 339		-25.038	43.521	1.00	0.00	3A7 3A7
ATOM	2382	0	LEU	339		-23.878 -25.565	43.325 44.752	1.00	0.00	3A7
ATOM	2383 2384	N CA	PRO	340 340		-24.851	45.907	1.00	0.00	3A7
ATOM ATOM	2385	CD	PRO PRO	340		-26.986	45.025	1.00	0.00	3A7
ATOM	2386	СВ	PRO	340		-25.968	46.840	1.00	0.00	3A7
ATOM	2387	CG	PRO	340		-27.154	46.523	1.00	0.00	3A7
ATOM	2388	С	PRO	340		-24.042	46.550	1.00	0.00	3A7
MOTA	2389	0	PRO	340		-24.463	46.512	1.00	0.00	3A7
MOTA	2390	N	ASN	341		-22.893	47.182	1.00	0.00	3A7
MOTA	2391	CA	ASN	341		-22.073	48.065	1.00	0.00	3A7
ATOM	2392	СВ	ASN	341		-22.872	49.244	1.00	0.00	3A7
ATOM	2393	CG	ASN	341		-23.614	50.023	1.00	0.00	3A7
ATOM	2394		ASN	341		-24.850	50.059	1.00	0.00	3A7
ATOM	2395		2 ASN	341		-22.826	50.663	1.00	0.00	3A7 3A7
ATOM	2396	C	ASN	341		-21.330 -20.897	47.312 46.178	1.00	0.00	3A7
ATOM ATOM	2397 2398	O N	ASN LYS	341 342		-20.897	47.953		0.00	3A7
ATOM	2399	CA	LYS	342		-20.529	47.396		0.00	3A7
MOTA	2400	CB	LYS	342		-19.456	48.339			3A7
ATOM	2401	CG	LYS	342		-18.309	48.647	1.00		3A7
ATOM	2402	CD	LYS	342		-17.205	49.527			3A7
ATOM	2403	CE	LYS			-17.674	50.944		0.00	3A7
MOTA	2404	NZ	LYS		10.133	-16.560	51.741	1.00	0.00	3A7

ATOM 2447 CB ASP 348 8.708 -34.785 38.996 1.00 0.00 3A7 ATOM 2448 CG ASP 348 9.678 -35.950 39.163 1.00 0.00 3A7 ATOM 2449 OD1 ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2450 OD2 ASP 348 10.439 -35.959 40.167 1.00 0.00 3A7 ATOM 2451 C ASP 348 7.939 -33.064 37.424 1.00 0.00 3A7 ATOM 2452 O ASP 348 6.884 -33.393 36.890 1.00 0.00 3A7 ATOM 2453 N, THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2454 CA THR 349 8.047 -29.394 38.153 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.047 -29.394 38.153 1.00 0.00 3A7 ATOM 2456 OG1 THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2458 C THR 349 7.246 -30.355 36.030 1.00 0.00 3A7 ATOM 2459 O THR 349 6.224 -29.855 35.582 1.00 0.00 3A7 ATOM 2460 N VAL 350 8.261 -30.585 33.760 1.00 0.00 3A7 ATOM 2461 CA VAL 350 8.261 -30.585 33.760 1.00 0.00 3A7 ATOM 2463 CG1 VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2463 CG1 VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 CG VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2467 N LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2469 CB LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2469 CB LEU 351 7.162 -36.712 34.024 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.066 -35.402 31.865 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.066 -35.402 31.865 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.066 -35.324 33.359 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.066 -35.324 33.359 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.062 -36.712 34.024 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.062 -36.712 34.024 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.062 -35.402 31.865 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00											
ATOM 2406 O LYS 342	ATOM	2405	С	LYS	342	10.016	-21.594	47.146	1.00	0.00	3A7
ATOM 2407 N ALA 343 9.595 -22.711 46.501 1.00 0.00 3A7 ATOM 2408 CA ALA 343 10.34 -23.539 46.171 1.00 0.00 3A7 ATOM 2410 C ALA 343 9.750 -25.189 46.76 1.00 0.00 3A7 ATOM 2411 C ALA 343 9.750 -25.189 44.700 1.00 0.00 3A7 ATOM 2411 N PRO 344 11.890 -24.000 44.274 1.00 0.00 3A7 ATOM 2412 N PRO 344 11.890 -24.000 44.274 1.00 0.00 3A7 ATOM 2412 C PRO 344 11.890 -24.000 44.274 1.00 0.00 3A7 ATOM 2415 CB PRO 344 11.890 -24.001 42.274 1.00 0.00 3A7 ATOM 2415 CB PRO 344 11.892 -24.012 42.880 1.00 0.00 3A7 ATOM 2415 CB PRO 344 11.892 -24.012 42.880 1.00 0.00 3A7 ATOM 2416 C PRO 344 11.892 -24.012 42.880 1.00 0.00 3A7 ATOM 2417 C PRO 344 11.892 -25.414 22.274 1.00 0.00 3A7 ATOM 2418 O PRO 345 11.880 -25.589 40.953 1.00 0.00 3A7 ATOM 2419 O PRO 345 11.880 -25.589 40.953 1.00 0.00 3A7 ATOM 2420 C PRO 345 11.205 -26.737 40.270 1.00 0.00 3A7 ATOM 2421 C PRO 345 11.680 -24.474 60.20 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.680 -24.474 60.20 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.402 -26.802 39.789 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.205 -26.737 40.270 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.402 -26.802 39.789 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.402 -24.802 39.789 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.402 -24.802 39.789 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.402 -24.802 39.789 1.00 0.00 3A7 ATOM 2422 C PRO 345 11.402 -29.156 40.280 1.00 0.00 3A7 ATOM 2424 C PRO 345 11.402 -29.156 40.280 1.00 0.00 3A7 ATOM 2427 C TA THR 346 11.432 -29.156 40.280 1.00 0.00 3A7 ATOM 2429 C TH 346 11.432 -29.156 40.280 1.00 0.00 3A7 ATOM 2429 C TH 346 11.432 -29.156 40.280 1.00 0.00 3A7 ATOM 2429 C TH 346 11.432 -29.156 40.280 1.00 0.00 3A7 ATOM 2430 C C THR 346 11.432 -39.133 40.280 1.00 0.00 3A7 ATOM 2431 C THR 346 11.432 -39.134 40.286 1.00 0.00 3A7 ATOM 2432 C THR 346 11.432 -39.135 1.00 0.00 3A7 ATOM 2430 C THR 346 11.432 -39.135 1.00 0.00 3A7 ATOM 2431 C THR 346 11.207 30.731 40.280 1.00 0.00 3A7 ATOM 2432 C THR 346 11.336 -31.339 1.00 0.00 3A7 ATOM 2436 C THR 346 11.336 -31.339 1.00 0.00 3A7 ATOM 2436 C THR 346 11.336 -33.339 1.00 0.00 3A7 ATOM 2436 C											
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ATOM 2412 N PRO 344 11.990 -24.000 44.274 1.00 0.00 3A7 ATOM 2414 CD PRO 344 13.149 -23.771 45.118 1.00 0.00 3A7 ATOM 2415 CB PRO 344 13.149 -23.771 45.118 1.00 0.00 3A7 ATOM 2416 CC PRO 344 11.399 -24.072 42.880 1.00 0.00 3A7 ATOM 2416 CC PRO 344 11.399 -24.072 42.880 1.00 0.00 3A7 ATOM 2416 CC PRO 344 11.20 -26.299 43.033 1.00 0.00 3A7 ATOM 2418 0 PRO 344 11.420 -26.299 43.033 1.00 0.00 3A7 ATOM 2418 N PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2419 N PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2420 CA PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2421 CD PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2427 C PRO 345 12.117 -27.995 40.521 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.329 -27.994 40.521 1.00 0.00 3A7 ATOM 2427 C A THR 346 11.432 -29.155 40.428 1.00 0.00 3A7 ATOM 2429 CG THR 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2429 CG THR 346 11.495 -31.522 41.180 1.00 0.00 3A7 ATOM 2431 C THR 346 11.495 -31.522 41.180 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.151 3B.32 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.551 3B.93 3B.95 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.551 3B.95 1.00 0.00 3A7 ATOM 2431 C THR 346 11.390 -30.551 3B.95 1.00 0.00 3A7 ATOM 2440 C EZ TTR 347 11.3830 -34.221 37.758 1.00 0.00 3A7 ATOM 2445 C B TR 347 11.3830 -34.221 37.585 1.00 0.00 3A7 ATOM 2446	MOTA	2410	С	ALA	343	10.737	-23.763	44.700	1.00	0.00	3A7
ATOM 2412 N PRO 344 11.980 -24.000 44.274 1.00 0.00 3A7 ATOM 2414 CD PRO 344 13.149 -23.771 45.118 1.00 0.00 3A7 ATOM 2415 CB PRO 344 13.149 -23.771 45.118 1.00 0.00 3A7 ATOM 2416 CG PRO 344 11.389 -24.072 42.880 1.00 0.00 3A7 ATOM 2416 CG PRO 344 11.289 -23.771 45.118 1.00 0.00 3A7 ATOM 2416 CG PRO 344 11.289 -23.514 42.274 1.00 0.00 3A7 ATOM 2418 0 PRO 344 11.290 -26.289 43.033 1.00 0.00 3A7 ATOM 2418 0 PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2419 N PRO 345 11.380 -25.589 40.533 1.00 0.00 3A7 ATOM 2420 CA PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2421 CD PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.295 -26.737 40.270 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.402 -26.392 3B.778 1.00 0.00 3A7 ATOM 2426 C PRO 345 11.329 -27.944 40.723 1.00 0.00 3A7 ATOM 2427 C A PRA 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2427 CA PRA 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2429 CG PRA 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2430 CG2 PRR 346 11.435 -31.522 41.180 1.00 0.00 3A7 ATOM 2431 C PRA 346 11.435 -31.522 41.180 1.00 0.00 3A7 ATOM 2431 C PRA 346 11.436 -39.983 3B.054 1.00 0.00 3A7 ATOM 2431 C PRA 346 11.336 -31.183 42.644 1.00 0.00 3A7 ATOM 2431 C PRA 346 11.336 -31.299 27.398 3B.054 1.00 0.00 3A7 ATOM 2431 C PRA 346 11.336 -31.339 3F.059 1.00 0.00 3A7 ATOM 2436 CG PRA 347 13.363 -33.809 3B.054 1.00 0.00 3A7 ATOM 2436 CG PRA 347 13.363 -33.809 3B.054 1.00 0.00 3A7 ATOM 2436 CG PRA 347 13.365 -33.809 3B.054 1.00 0.00 3A7 ATOM 2440 CEZ PTR 347 13.363 -34.221 37.588 1.00 0.00 3A7 ATOM 2440 CEZ PTR 347 13.363 -33.809 3B.054 1.00 0.00 3A7 ATOM 2440 CEZ PTR 347 13.363 -33.809 3B.054 1.00 0.00 3A7 ATOM 2440 CEZ PTR 347 14.690 -33.809 3B.054 1.00 0.00 3A7 ATOM 2445 C A PRA 349 348 9.034 -32.995 39.535 1.00	ATOM	2411	0	ALA	343	9.824	-23.520	43.911	1.00	0.00	3A7
ATOM 2413 CA PRO 344 12.553 -24.110 42.875 1.00 0.00 3A7 ATOM 2415 CB PRO 344 13.894 -24.072 42.880 1.00 0.00 3A7 ATOM 2416 CG PRO 344 11.2838 -25.414 42.274 1.00 0.00 3A7 ATOM 2417 C PRO 344 11.2838 -25.414 42.274 1.00 0.00 3A7 ATOM 2418 0 PRO 344 11.2838 -25.414 42.274 1.00 0.00 3A7 ATOM 2419 N PRO 345 11.880 -25.589 40.953 1.00 0.00 3A7 ATOM 2419 N PRO 345 11.880 -25.589 40.953 1.00 0.00 3A7 ATOM 2412 CD PRO 345 11.880 -25.589 40.953 1.00 0.00 3A7 ATOM 2421 CD PRO 345 11.880 -25.589 40.953 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.252 -26.737 40.270 1.00 0.00 3A7 ATOM 2421 CD PRO 345 11.402 -26.382 3B.778 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.402 -26.382 3B.778 1.00 0.00 3A7 ATOM 2425 CB PRO 345 11.402 -26.382 3B.731 1.00 0.00 3A7 ATOM 2425 CB PRO 345 11.402 -26.382 3B.731 1.00 0.00 3A7 ATOM 2425 CB PRO 345 11.402 -26.382 3B.731 1.00 0.00 3A7 ATOM 2425 CB PRO 345 11.402 -26.382 3B.731 1.00 0.00 3A7 ATOM 2425 CB PRO 345 11.402 -26.382 3B.731 1.00 0.00 3A7 ATOM 2425 CB PRO 345 13.329 -27.934 40.723 1.00 0.00 3A7 ATOM 2425 CB TRIM 346 11.432 -29.155 40.428 1.00 0.00 3A7 ATOM 2425 CB TRIM 346 11.432 -29.155 40.428 1.00 0.00 3A7 ATOM 2420 CG TRIM 346 10.071 -31.633 41.047 1.00 0.00 3A7 ATOM 2420 CG TRIM 346 10.071 -31.633 41.047 1.00 0.00 3A7 ATOM 2430 CG TRIM 346 10.071 -31.633 41.047 1.00 0.00 3A7 ATOM 2431 CC TRIM 346 11.280 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 CC TRIM 346 11.280 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 CC TRIM 346 11.280 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 CC TRIM 346 11.360 -39.93 3B.055 1.00 0.00 3A7 ATOM 2431 CC TRIM 346 11.360 -39.93 3B.055 1.00 0.00 3A7 ATOM 2432 C TRIM 346 11.360 -39.93 3B.055 1.00 0.00 3A7 ATOM 2435 CB TYM 347 13.245 -32.298 37.025 1.00 0.00 3A7 ATOM 2435 CB TYM 347 13.245 -32.298 37.025 1.00 0.00 3A7 ATOM 2435 CB TYM 347 13.245 -32.298 37.025 1.00 0.00 3A7 ATOM 2435 CB TYM 347 13.266 -35.455 3B.007 1.00 0.00 3A7 ATOM 2435 CB TYM 347 13.266 -35.455 3B.007 1.00 0.00 3A7 ATOM 2445 CG TYM 347 13.266 -35.455 3B.007 1.00 0.00 3A7 ATOM 2455 CG TYM 347 13.266 -35.455 3B.007 1.									1.00		3A7
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ATOM 2418 O PRO 344 11.420 -26.289 43.033 1.00 0.00 3A7 ATOM 2420 CA PRO 345 11.880 -25.589 40.095 1.00 0.00 3A7 ATOM 2421 CD PRO 345 11.880 -25.589 40.003 1.00 0.00 3A7 ATOM 2422 CG PRO 345 11.298 -24.479 40.003 1.00 0.00 3A7 ATOM 2422 CG PRO 345 11.412 -24.857 3B.3711 1.00 0.00 3A7 ATOM 2423 CG PRO 345 11.412 -24.857 3B.3711 1.00 0.00 3A7 ATOM 2424 C PRO 345 12.117 -27.996 40.521 1.00 0.00 3A7 ATOM 2425 O PRO 345 12.117 -27.996 40.521 1.00 0.00 3A7 ATOM 2426 N THR 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2427 CA THR 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2428 CB THR 346 11.495 -31.522 41.180 1.00 0.00 3A7 ATOM 2429 CB THR 346 11.495 -31.523 41.180 1.00 0.00 3A7 ATOM 2429 CB THR 346 11.330 -31.183 41.047 1.00 0.00 3A7 ATOM 2429 CC THR 346 11.330 -31.183 41.047 1.00 0.00 3A7 ATOM 2429 CC THR 346 11.330 -31.183 42.041 1.00 0.00 3A7 ATOM 2420 CT THR 346 11.330 -31.183 41.047 1.00 0.00 3A7 ATOM 2430 CC2 THR 346 11.330 -31.183 40.047 1.00 0.00 3A7 ATOM 2431 CT THR 346 11.346 -9.983 38.054 1.00 0.00 3A7 ATOM 2432 O THR 346 11.346 -9.983 38.054 1.00 0.00 3A7 ATOM 2433 C THR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2434 CA TTR 347 12.345 -32.298 37.022 1.00 0.00 3A7 ATOM 2435 CB TYR 347 13.830 -34.221 37.788 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.830 -34.221 37.788 1.00 0.00 3A7 ATOM 2437 CDI TYR 347 13.830 -34.221 37.788 1.00 0.00 3A7 ATOM 2440 CG TYR 347 13.830 -34.221 37.788 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 13.630 -36.639 80.050 1.00 0.00 3A7 ATOM 2443 C CT TYR 347 13.630 -36.639 80.050 1.00 0.00 3A7 ATOM 2440 CE2 TYR 347 13.630 -36.639 80.050 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 13.630 -36.639 80.050 1.00 0.00 3A7 ATOM 2445 C B TYR 347 13.630 -36.639 80.050 1.00 0.00 3A7 ATOM 2446 C C TYR 347 13.630 -36.639 80.050 1.00 0.00 3A7 ATOM 2447 C B ASP 348 8.068 -33.809 38.641 1.00 0.00 3A7 ATOM 2446 C C TYR 347 13.630 -36.639 30.00 1.00 0.00 3A7 ATOM 2447 C B ASP 348 8.000 3.000 3A7 ATOM 2455 C B THR 349 8.000 3.000 3A7 ATOM 2456 C TYR 347 10.936 3.000 3A7 ATOM 2457 C C THR 349 8.000 3A7 ATOM 2458 C THR 349	ATOM	2417	С	PRO	344	11.838	-25.414	42.274	1.00	0.00	3A7
ATOM 2419 N PRO 345 11.385 -25.589 40.953 1.00 0.00 3A7 ATOM 2421 CD PRO 345 11.325 -26.737 40.270 1.00 0.00 3A7 ATOM 2422 CB PRO 345 11.00 12.00 0.00 3A7 ATOM 2422 CB PRO 345 11.402 -26.382 3B.778 1.00 0.00 3A7 ATOM 2423 CG PRO 345 11.402 -24.857 3B.778 1.00 0.00 3A7 ATOM 2424 CP PRO 345 11.402 -24.857 3B.718 1.00 0.00 3A7 ATOM 2425 C PRO 345 11.402 -24.857 3B.718 1.00 0.00 3A7 ATOM 2426 N THR 346 11.325 -27.996 40.521 1.00 0.00 3A7 ATOM 2427 CA THR 346 11.322 -27.996 40.521 1.00 0.00 3A7 ATOM 2428 CB THR 346 11.322 -27.914 40.723 1.00 0.00 3A7 ATOM 2428 CB THR 346 11.325 -27.915 40.428 1.00 0.00 3A7 ATOM 2428 CB THR 346 11.325 -27.915 40.428 1.00 0.00 3A7 ATOM 2429 CG1 THR 346 10.071 -31.633 41.047 1.00 0.00 3A7 ATOM 2431 C THR 346 11.920 -30.751 3B.827 1.00 0.00 3A7 ATOM 2432 O THR 346 11.920 -30.751 3B.827 1.00 0.00 3A7 ATOM 2432 O THR 346 11.920 -30.751 3B.827 1.00 0.00 3A7 ATOM 2432 C THR 346 11.920 -30.751 3B.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.920 -30.751 3B.807 10.00 0.00 3A7 ATOM 2432 C THR 346 11.920 -30.751 3B.807 10.00 0.00 3A7 ATOM 2431 C THR 346 11.3345 -32.298 37.022 1.00 0.00 3A7 ATOM 2432 C THR 347 12.422 -31.922 3B.605 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.345 -32.298 37.022 1.00 0.00 3A7 ATOM 2439 CE TYR 347 13.345 -33.983 36.599 1.00 0.00 3A7 ATOM 2439 CE TYR 347 13.935 -35.555 3B.007 1.00 0.00 3A7 ATOM 2439 CE TYR 347 13.633 -36.258 39.060 1.00 0.00 3A7 ATOM 2440 CE TYR 347 13.633 -36.258 39.060 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 11.636 3.36.258 39.060 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 11.636 3.36.258 39.060 1.00 0.00 3A7 ATOM 2442 CH TYR 347 13.633 -36.258 39.060 1.00 0.00 3A7 ATOM 2445 C ASP 348 8.768 -35.855 38.697 1.00 0.00 3A7 ATOM 2446 CA ASP 348 8.768 -35.855 38.007 1.00 0.00 3A7 ATOM 2446 CA ASP 348 8.768 -35.855 38.696 1.00 0.00 3A7 ATOM 2446 C ASP 348 8.768 -35.855 38.696 1.00 0.00 3A7 ATOM 2446 C ASP 348 8.768 -35.855 38.696 1.00 0.00 3A7 ATOM 2446 C C ASP 348 8.768 -35.855 38.697 1.00 0.00 3A7 ATOM 2446 C C ANL 350 8.686 38.698 39.308 1.00 0.00 3A7 ATOM 2446 C C ANL 350 8	ATOM	2418	0	PRO	344	11.420	-26.289	43.033	1.00	0.00	3A7
ATOM 2420 CA PRO 345 11.325 -26.737 40.270 1.00 0.00 3A7 ATOM 2421 CD PRO 345 12.098 -24.479 40.003 1.00 0.00 .00 ATOM 2422 CG PRO 345 11.402 -24.897 38.731 1.00 0.00 3A7 ATOM 2423 CG PRO 345 11.412 -24.897 38.731 1.00 0.00 3A7 ATOM 2424 C PRO 345 11.412 -24.897 38.731 1.00 0.00 3A7 ATOM 2425 O PRO 345 12.117 -27.996 40.521 1.00 0.00 3A7 ATOM 2426 N THR 346 11.432 -92.9156 40.521 1.00 0.00 3A7 ATOM 2427 CA THR 346 11.432 -92.9156 40.288 1.00 0.00 3A7 ATOM 2427 CA THR 346 11.432 -92.9156 40.628 1.00 0.00 3A7 ATOM 2429 CG THR 346 11.485 -31.522 41.189 1.00 0.00 3A7 ATOM 2429 O THR 346 11.895 -31.183 41.047 1.00 0.00 3A7 ATOM 2430 CC THR 346 11.930 -31.183 42.644 1.00 0.00 3A7 ATOM 2431 C THR 346 11.392 -30.751 38.827 1.00 0.00 3A7 ATOM 2432 O THR 346 11.346 -9.9983 38.054 1.00 0.00 3A7 ATOM 2431 C THR 346 11.346 -9.9983 38.054 1.00 0.00 3A7 ATOM 2433 N TYR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2434 CA TYR 347 12.345 -32.298 37.022 1.00 0.00 3A7 ATOM 2435 CB TYR 347 13.345 -33.383 36.599 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2437 CD TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2438 CB TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2439 CB TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2439 CB TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2439 CB TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2439 CB TYR 347 15.130 -34.609 39.638 1.00 0.00 3A7 ATOM 2439 CB TYR 347 15.130 -34.609 39.638 1.00 0.00 3A7 ATOM 2439 CB TYR 347 15.130 -34.609 39.638 1.00 0.00 3A7 ATOM 2430 CB TYR 347 16.967 -35.835 39.060 1.00 0.00 3A7 ATOM 2437 CB TYR 347 16.967 -35.835 39.060 1.00 0.00 3A7 ATOM 2440 CB TYR 347 10.471 -32.653 35.655 1.00 0.00 3A7 ATOM 2440 CB TYR 347 15.130 -34.609 39.638 1.00 0.00 3A7 ATOM 2440 CB TYR 347 10.347 1-32.653 35.655 1.00 0.00 3A7 ATOM 2440 CB TYR 347 10.347 1-32.653 35.655 1.00 0.00 3A7 ATOM 2440 CB TYR 347 10.347 1-32.653 35.655 1.00 0.00 3A7 ATOM 2450 CB TYR 349 1.00 3A8 3.348 3.348 3.359 1.00 0.00 3A7 ATOM 2450 CB TYR 349 348 8.005 3.399 3.300 0.00		2419				11 880	-25.589			0.00	3A7
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ATOM 2426 N THR 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2427 CA THR 346 12.073 -30.434 40.286 1.00 0.00 3A7 ATOM 2428 CB THR 346 11.432 -29.156 40.428 1.00 0.00 3A7 ATOM 2429 CGI THR 346 11.435 -31.522 41.18p 1.00 0.00 3A7 ATOM 2430 CG2 THR 346 11.85 -31.522 41.18p 1.00 0.00 3A7 ATOM 2431 C THR 346 11.80 -31.183 42.644 1.00 0.00 3A7 ATOM 2431 C THR 346 11.80 -31.183 42.644 1.00 0.00 3A7 ATOM 2432 O THR 346 11.920 -30.751 38.827 1.00 0.00 3A7 ATOM 2432 O THR 346 11.346 -29.983 38.054 1.00 0.00 3A7 ATOM 2433 N TYR 347 12.345 -32.288 37.022 1.00 0.00 3A7 ATOM 2434 CA TYR 347 12.345 -32.288 37.022 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.345 -33.383 36.559 1.00 0.00 3A7 ATOM 2437 CDI TYR 347 13.226 -35.455 38.007 1.00 0.00 3A7 ATOM 2438 CDZ TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2439 CEI TYR 347 13.680 -34.221 37.758 1.00 0.00 3A7 ATOM 2439 CEI TYR 347 13.680 -34.629 39.660 1.00 0.00 3A7 ATOM 2440 CEZ TYR 347 13.680 -34.699 39.638 1.00 0.00 3A7 ATOM 2440 CEZ TYR 347 14.680 -33.809 38.584 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 14.680 -33.809 38.584 1.00 0.00 3A7 ATOM 2442 OH TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2442 CH TYR 347 14.697 -35.835 39.807 1.00 0.00 3A7 ATOM 2444 C TYR 347 10.966 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 C TYR 347 10.966 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 C A TYR 347 10.966 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 C A SP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2445 C A SP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2447 CB ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2445 C A SP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2446 CA THR 349 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2455 C B THR 349 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2456 C THR 349 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2457 C C BASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2458 C THR 349 9.665 -36.846 38.103 1.00 0.00 3A7 ATOM 2456 C C THR 349 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2457 C C BR 349 9.665 -36.846 38.103 31.00 0.00 3A7 ATOM	MOTA	2425	0	PRO	345	13.329	-27.934	40.723	1.00	0.00	3A7
ATOM 2428 CB THR 346 12.073 -30.434 40.286 1.00 0.00 3A7 ATOM 2428 CB THR 346 11.485 -31.522 41.180 1.00 0.00 3A7 ATOM 2429 OG1 THR 346 11.091 -31.633 41.047 1.00 0.00 3A7 ATOM 2430 CG2 THR 346 11.930 -31.183 42.644 1.00 0.00 3A7 ATOM 2431 C THR 346 11.920 -30.751 38.827 1.00 0.00 3A7 ATOM 2431 C THR 346 11.920 -30.751 38.827 1.00 0.00 3A7 ATOM 2432 O THR 346 11.920 -30.751 38.827 1.00 0.00 3A7 ATOM 2433 N TYR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2433 N TYR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2435 CB TYR 347 13.455 -32.298 37.022 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.455 -32.298 37.022 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.465 -33.833 36.599 1.00 0.00 3A7 ATOM 2436 CD TYR 347 13.863 -34.221 37.758 1.00 0.00 3A7 ATOM 2438 CD2 TYR 347 13.863 -34.221 37.758 1.00 0.00 3A7 ATOM 2438 CD2 TYR 347 13.863 -33.833 36.599 1.00 0.00 3A7 ATOM 2439 CEI TYR 347 13.863 -36.258 39.060 1.00 0.00 3A7 ATOM 2431 CZ TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.313 -36.649 40.945 1.00 0.00 3A7 ATOM 2442 CH TYR 347 15.313 -36.649 40.945 1.00 0.00 3A7 ATOM 2445 N ASP 348 10.354 -33.847 37.746 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.068 -33.895 39.996 1.00 0.00 3A7 ATOM 2445 N ASP 348 9.068 -33.895 39.996 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.068 -33.895 39.996 1.00 0.00 3A7 ATOM 2457 CB ASP 348 9.068 -33.895 39.996 1.00 0.00 3A7 ATOM 2458 CC THR 349 9.678 -33.959 39.163 1.00 0.00 3A7 ATOM 2459 OT ASP 348 9.068 -36.846 38.277 1.00 0.00 3A7 ATOM 2456 CG THR 349 9.662 -36.846 38.277 1.00 0.00 3A7 ATOM 2457 CC ASP 348 9.068 -36.846 38.277 1.00 0.00 3A7 ATOM 2458 CC THR 349 9.068 -36.846 38.277 1.00 0.00 3A7 ATOM 2459 CC THR 349 9.068 -32.842 30.595 1.00 0.00 3A7 ATOM 2456 CC THR 349 9.068 -32.842 30.008 31.00 0.00 3A7 ATOM 2466											
ATOM 2428 CB THR 346 11.485 -31.522 41.180 1.00 0.00 3A7											
ATOM 2429 OG1 THR 346											
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ATOM 2431 C THR 346 11.320 -30.751 38.827 1.00 0.00 3A7 ATOM 2432 O THR 346 11.346 -29.983 38.054 1.00 0.00 3A7 ATOM 2433 N TYR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2435 CB TYR 347 12.345 -32.298 37.022 1.00 0.00 3A7 ATOM 2435 CB TYR 347 13.345 -33.383 36.599 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.835 -33.383 36.599 1.00 0.00 3A7 ATOM 2437 CD1 TYR 347 13.836 -33.4221 37.758 1.00 0.00 3A7 ATOM 2438 CD2 TYR 347 13.836 -33.4221 37.758 1.00 0.00 3A7 ATOM 2438 CD2 TYR 347 13.653 -36.258 39.060 1.00 0.00 3A7 ATOM 2439 CE1 TYR 347 13.653 -36.258 39.060 1.00 0.00 3A7 ATOM 2439 CE1 TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.131 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.133 -36.649 40.945 1.00 0.00 3A7 ATOM 2444 O TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 O TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 O TYR 347 10.471 -32.653 35.655 1.00 0.00 3A7 ATOM 2444 C A ASP 348 10.354 -33.487 37.764 1.00 0.00 3A7 ATOM 2446 CA ASP 348 8.708 34.909 39.638 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.0678 -35.835 99.163 1.00 0.00 3A7 ATOM 2447 CB ASP 348 9.0678 -35.959 39.163 1.00 0.00 3A7 ATOM 2449 ODI ASP 348 9.678 -35.959 39.163 1.00 0.00 3A7 ATOM 2449 ODI ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2445 N ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2450 ODZ ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.414 -30.615 37.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.414 -30.615 37.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.424 -30.515 37.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.424 -30.515 37.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.424 -30.515 37.512 1.00 0.00 3A7 ATOM 2458 CG THR 349 7.424 -30.515 37.512 1.00 0.00 3A7 ATOM 2459 CG THR 349 7.426 -30.355 36.000 1.00 0.00 3A7 ATOM 2460 N VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2467 CG VAL 350 9.700 -31.257 31.710 0.00 0.00 3A7 ATOM	ATOM	2429	OG1	THR							
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ATOM 2431 N TYR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2435 CB TYR 347 12.345 -32.298 37.022 1.00 0.00 .3A7 ATOM 2435 CB TYR 347 13.345 -33.383 36.599 1.00 0.00 .3A7 ATOM 2436 CG TYR 347 13.830 -34.221 37.758 1.00 0.00 .3A7 ATOM 2437 CDI TYR 347 13.830 -34.221 37.758 1.00 0.00 .3A7 ATOM 2438 CD2 TYR 347 14.880 -33.809 38.584 1.00 0.00 .3A7 ATOM 2439 CEI TYR 347 15.310 -34.609 39.638 1.00 0.00 .3A7 ATOM 2440 CE2 TYR 347 15.310 -34.609 39.638 1.00 0.00 .3A7 ATOM 2441 CZ TYR 347 14.697 -35.835 39.877 1.00 0.00 .3A7 ATOM 2442 OH TYR 347 10.986 -32.842 36.741 1.00 0.00 .3A7 ATOM 2444 CT TYR 347 10.471 -32.653 35.655 1.00 0.00 .3A7 ATOM 2444 OT TYR 347 10.471 -32.653 35.655 1.00 0.00 .3A7 ATOM 2445 N ASP 348 10.354 -33.487 37.746 1.00 0.00 .3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 .3A7 ATOM 2447 CB ASP 348 9.033 -34.072 37.677 1.00 0.00 .3A7 ATOM 2449 ODI ASP 348 9.665 -36.846 38.277 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 9.665 -36.846 38.277 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2451 C ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 90.103 1.00 0.00 .3A7 ATOM 2451 C ASP 348 6.849 -33.393 36.69 0.00 0.00 .3A7 ATOM 2452 O ASP 348 6.849 -33.393 36.69 0.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 6.849 -33.393 36.60 0.00 0.00 .3A7 ATOM 2451 C ASP 348 6.849 -33.393 36.60 0.00 0.00 .3A7 ATOM 2452 O ASP 348 6.849 -33.393 36.60 0.00 0.00 .3A7 ATOM 2454 C A THR 349 8.047 -29.394 38.153 1.00 0.00 .3A7 ATOM 2456 C B THR 349 8.047 -29.395 33.595 1.00 0.00 .3A7 ATOM 2457 CG2 THR 349 8.047 -29.395 33.595 1.00 0.00 .3A7 ATOM 2466 C C VAL 350 6.691 -30.900 31.900 0.00 .3A7 ATOM 2467 N LEU 351 5.683 -33.220 33.054 1.00 0.00 .3A7 ATOM 2468 C C VAL 350 7	ATOM	2431	С	THR	346	11.920	-30.751	38.827	1.00	0.00	3A7
ATOM 2434 CA TYR 347 12.422 -31.922 38.405 1.00 0.00 3A7 ATOM 2435 CB TYR 347 12.345 -32.298 37.022 1.00 0.00 .3A7 ATOM 2436 CG TYR 347 13.345 -33.383 36.599 1.00 0.00 .3A7 ATOM 2436 CG TYR 347 13.830 -34.221 37.758 1.00 0.00 .3A7 ATOM 2438 CD2 TYR 347 13.830 -34.221 37.758 1.00 0.00 .3A7 ATOM 2438 CD2 TYR 347 14.880 -33.809 38.584 1.00 0.00 .3A7 ATOM 2439 CE1 TYR 347 15.310 -34.609 39.638 1.00 0.00 .3A7 ATOM 2440 CE2 TYR 347 15.310 -34.609 39.638 1.00 0.00 .3A7 ATOM 2441 CZ TYR 347 14.697 -35.835 39.877 1.00 0.00 .3A7 ATOM 2441 CZ TYR 347 10.986 -32.842 36.741 1.00 0.00 .3A7 ATOM 2444 CT TYR 347 10.986 -32.842 36.741 1.00 0.00 .3A7 ATOM 2445 N ASP 348 10.354 -33.487 37.746 1.00 0.00 .3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 .3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 .3A7 ATOM 2447 CB ASP 348 8.708 -34.785 38.996 1.00 0.00 .3A7 ATOM 2446 CA ASP 348 9.665 -36.846 38.277 1.00 0.00 .3A7 ATOM 2445 N ASP 348 9.665 -36.846 38.277 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 9.665 -36.846 38.277 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 40.167 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 10.439 -335.959 40.167 1.00 0.00 .3A7 ATOM 2451 C ASP 348 17.439 -33.999 40.167 1.00 0.00 .3A7 ATOM 2452 O ASP 348 10.439 -335.959 40.167 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 8.684 -33.393 36.69 0.00 0.00 .3A7 ATOM 2451 C ASP 348 6.849 -33.393 36.809 1.00 0.00 .3A7 ATOM 2452 O ASP 348 8.9665 -36.846 38.277 1.00 0.00 .3A7 ATOM 2450 OD2 ASP 348 6.884 -33.393 36.80 0.00 0.00 .3A7 ATOM 2451 C ASP 348 6.849 -33.393 36.80 0.00 0.00 .3A7 ATOM 2452 O ASP 348 6.849 -33.393 36.80 0.00 0.00 .3A7 ATOM 2454 CA THR 349 8.224 -31.784 37.764 1.00 0.00 .3A7 ATOM 2455 CB THR 349 8.047 -29.394 38.153 1.00 0.00 .3A7 ATOM 2456 CG THR 349 8.047 -29.395 33.595 0.00 0.00 .3A7 ATOM 2457 CG THR 349 8.047 -29.395 33.595 0.00 0.00 .3A7 ATOM 2456 CG THR 349 8.047 -29.395 33.595 0.00 0.00 .3A7 ATOM 2457 CG THR 349 8.047 -29.395 33.595 0.00 0.00 .3A7 ATOM 2466 CG VAL 350 7.128 -31.305 33.595 1.00 0.00 .3A7 ATOM 2467 CG LEU 351 5.689 -34.682	ATOM	2432	0	THR	346	11.346	-29.983	38.054	1.00	0.00	3A7
ATOM 2435 CB TYR 347 13.345 -32.298 37.022 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2436 CG TYR 347 13.830 -34.221 37.758 1.00 0.00 3A7 ATOM 2438 CDZ TYR 347 13.226 -35.455 38.007 1.00 0.00 3A7 ATOM 2438 CDZ TYR 347 13.653 -36.258 39.060 1.00 0.00 3A7 ATOM 2439 CEI TYR 347 13.653 -36.258 39.060 1.00 0.00 3A7 ATOM 2440 CEZ TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 15.133 -36.649 40.945 1.00 0.00 3A7 ATOM 2442 OH TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 O TYR 347 10.471 -32.653 35.655 1.00 0.00 3A7 ATOM 2445 C TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.746 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.746 1.00 0.00 3A7 ATOM 2448 CG ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2449 ODI ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2449 ODI ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2450 ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2451 C ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2451 C ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2451 C ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2452 O ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2454 CA THR 349 7.939 -33.064 37.424 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.224 -31.784 37.754 1.00 0.00 3A7 ATOM 2456 ORI THR 349 8.244 -31.784 37.754 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 8.047 -29.394 38.153 1.00 0.00 3A7 ATOM 2458 C THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2456 ORI THR 349 8.244 -31.784 37.764 1.00 0.00 3A7 ATOM 2456 CB THR 349 7.246 -30.355 36.030 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.246 -30.355 36.030 1.00 0.00 3A7 ATOM 2458 C THR 349 7.246 -30.355 33.760 1.00 0.00 3A7 ATOM 2456 CB VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2466 CB VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2467 CG EU 351 5.689 -34.682 33.359 1.00 0.00 3A7 ATOM 2468 CB VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2468 CB VAL 350 9.589 -31.111 33.250 1.00 0.00 3A7 ATOM 2469 CB LEU 351									1.00	0.00	3A7
ATOM 2436 CG TYR 347 13.345 -33.383 36.599 1.00 0.00 3A7 ATOM 2437 CD1 TYR 347 13.826 -33.455 38.007 1.00 0.00 .3A7 ATOM 2438 CD2 TYR 347 14.880 -33.809 38.584 1.00 0.00 3A7 ATOM 2439 CD1 TYR 347 15.510 -34.609 38.584 1.00 0.00 3A7 ATOM 2440 CE2 TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 14.697 -35.835 39.877 1.00 0.00 3A7 ATOM 2442 CH TYR 347 15.310 -34.609 39.638 1.00 0.00 3A7 ATOM 2442 CH TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2442 CH TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2443 C TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 CH TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2445 CH TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2446 CA ASP 348 10.354 -33.487 37.746 1.00 0.00 3A7 ATOM 2447 CB ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2448 CG ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2449 OLD ASP 348 9.678 -35.950 39.163 1.00 0.00 3A7 ATOM 2449 OLD ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2450 CD ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2451 C ASP 348 10.439 -35.959 40.167 1.00 0.00 3A7 ATOM 2452 O ASP 348 10.439 -35.959 40.167 1.00 0.00 3A7 ATOM 2453 C THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2454 CT ASP 348 6.884 -33.393 36.690 1.00 0.00 3A7 ATOM 2450 OD ASP 348 6.884 -33.393 36.690 1.00 0.00 3A7 ATOM 2451 C ASP 348 6.884 -33.393 36.809 0.00 0.00 3A7 ATOM 2452 O ASP 348 6.884 -33.393 36.809 0.00 0.00 3A7 ATOM 2454 CT THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2456 CG THR 349 8.244 -31.784 37.764 1.00 0.00 3A7 ATOM 2457 CGZ THR 349 7.114 -30.615 37.512 1.00 0.00 3A7 ATOM 2456 CG THR 349 8.244 -31.784 37.764 1.00 0.00 3A7 ATOM 2457 CGZ THR 349 7.144 -30.615 37.512 1.00 0.00 3A7 ATOM 2458 C THR 349 7.146 -30.355 36.030 1.00 0.00 3A7 ATOM 2457 CGZ THR 349 7.146 -30.355 36.030 1.00 0.00 3A7 ATOM 2458 C THR 349 7.246 -30.355 36.030 1.00 0.00 3A7 ATOM 2457 CGZ THR 349 7.146 -30.388 33.599 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.683 -33.220 33.599 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2468 CA											
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ATOM 2440 CE2 TYR 347	ATOM	2438	CD2	TYR	347	14.880	-33.809	38.584	1.00	0.00	3A7
ATOM 2441 CZ TYR 347 14.697 -35.835 39.877 1.00 0.00 3A7 ATOM 2441 CZ TYR 347 14.697 -35.835 39.877 1.00 0.00 3A7 ATOM 2442 OH TYR 347 15.133 -36.649 40.945 1.00 0.00 3A7 ATOM 2443 C TYR 347 10.986 -32.842 36.741 1.00 0.00 3A7 ATOM 2444 O TYR 347 10.471 -32.653 35.655 1.00 0.00 3A7 ATOM 2445 N ASP 348 10.354 -33.487 37.746 1.00 0.00 3A7 ATOM 2446 CA ASP 348 9.033 -34.072 37.677 1.00 0.00 3A7 ATOM 2447 CB ASP 348 8.708 -34.785 38.996 1.00 0.00 3A7 ATOM 2449 OD1 ASP 348 9.678 -35.950 39.163 1.00 0.00 3A7 ATOM 2449 OD1 ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2450 OD2 ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2451 C ASP 348 9.686 -36.846 38.277 1.00 0.00 3A7 ATOM 2452 O ASP 348 6.884 -33.393 36.890 1.00 0.00 3A7 ATOM 2453 N THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.224 -31.784 37.564 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2456 OG1 THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2456 OG1 THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2458 C THR 349 7.246 -30.355 35.585 1.00 0.00 3A7 ATOM 2459 O THR 349 6.244 -30.615 37.512 1.00 0.00 3A7 ATOM 2450 OVAL 350 8.243 -30.735 35.503 1.00 0.00 3A7 ATOM 2456 OG1 THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2456 OG THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2460 N VAL 350 8.243 -30.735 35.503 1.00 0.00 3A7 ATOM 2467 N LEU 351 5.689 -31.111 33.245 1.00 0.00 3A7 ATOM 2467 N LEU 351 5.689 -31.217 33.359 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2469 CB LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2467 N LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2467 N LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.046 -35.324 33.359 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.62 -36.712 34.024 1.00 0.00 3A7 ATOM 2471 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 7.441 -35	ATOM	2439	CE1	TYR	347	13.653	-36.258	39.060	1.00	0.00	3A7
ATOM 2441 CZ TYR 347								39.638	1.00	0.00	3A7
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ATOM 2448 CG ASP 348 9.678 -35.950 39.163 1.00 0.00 3A7 ATOM 2449 OD1 ASP 348 9.665 -36.846 38.277 1.00 0.00 3A7 ATOM 2450 OD2 ASP 348 10.439 -35.959 40.167 1.00 0.00 3A7 ATOM 2451 C ASP 348 7.939 -33.064 37.424 1.00 0.00 3A7 ATOM 2452 O ASP 348 6.884 -33.393 36.890 1.00 0.00 3A7 ATOM 2453 N THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2453 N THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.047 -29.394 38.153 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.047 -29.394 38.153 1.00 0.00 3A7 ATOM 2455 CG THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2458 C THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2458 C THR 349 7.246 -30.355 36.030 1.00 0.00 3A7 ATOM 2459 O THR 349 6.224 -29.855 35.582 1.00 0.00 3A7 ATOM 2450 N VAL 350 8.241 -30.585 33.760 1.00 0.00 3A7 ATOM 2460 N VAL 350 8.241 -30.585 33.760 1.00 0.00 3A7 ATOM 2462 CB VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2462 CB VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2464 CG2 VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2465 C VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2466 N VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.589 -31.273 33.764 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C LEU 351 6.619 -32.397 33.667 1.00 0.00 3A7 ATOM 2467 C LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2467 C LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0	MOTA	2446	CA	ASP	348	9.033	-34.072	37.677	1.00	0.00	3A7
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ATOM 2450 OD2 ASP 348										0.00	3A7
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ATOM 2451 C ASP 348 7.939 -33.064 37.424 1.00 0.00 3A7 ATOM 2452 O ASP 348 6.884 -33.393 36.890 1.00 0.00 3A7 ATOM 2453 N THR 349 8.224 -31.784 37.764 1.00 0.00 3A7 ATOM 2454 CA THR 349 7.414 -30.615 37.512 1.00 0.00 3A7 ATOM 2455 CB THR 349 8.047 -29.394 38.153 1.00 0.00 3A7 ATOM 2456 OG1 THR 349 8.345 -29.682 39.512 1.00 0.00 3A7 ATOM 2457 CG2 THR 349 7.118 -28.168 38.103 1.00 0.00 3A7 ATOM 2458 C THR 349 7.246 -30.355 36.030 1.00 0.00 3A7 ATOM 2459 O THR 349 6.224 -29.855 35.582 1.00 0.00 3A7 ATOM 2450 N VAL 350 8.243 -30.735 35.203 1.00 0.00 3A7 ATOM 2461 CA VAL 350 8.261 -30.585 33.760 1.00 0.00 3A7 ATOM 2462 CB VAL 350 9.589 -31.111 33.245 1.00 0.00 3A7 ATOM 2463 CG1 VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 9.700 -31.257 31.710 1.00 0.00 3A7 ATOM 2466 C VAL 350 6.691 -30.988 33.784 1.00 0.00 3A7 ATOM 2466 C VAL 350 6.691 -30.900 31.980 1.00 0.00 3A7 ATOM 2466 C VAL 350 6.691 -30.900 31.980 1.00 0.00 3A7 ATOM 2466 C A LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2467 N LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2467 CG LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.162 -36.712 34.024 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00											
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ATOM 2456 OG1 THR 349	MOTA	2454	CA	THR	349	7.414	-30.615	37.512	1.00	0.00	3A7
ATOM 2456 OG1 THR 349	ATOM	2455	CB	THR	349	8.047	-29.394	38.153	1.00	0.00	3A7
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ATOM 2464 CG2 VAL 350 10.704 -30.188 33.784 1.00 0.00 3A7 ATOM 2465 C VAL 350 7.128 -31.305 33.054 1.00 0.00 3A7 ATOM 2466 O VAL 350 6.691 -30.900 31.980 1.00 0.00 3A7 ATOM 2467 N LEU 351 6.619 -32.397 33.667 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2469 CB LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 4.203 -32.710 33.432 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00	ATOM	2462	СВ	VAL	350	9.589	-31.111	33.245	1.00	0.00	3A7
ATOM 2464 CG2 VAL 350 10.704 -30.188 33.784 1.00 0.00 3A7 ATOM 2465 C VAL 350 7.128 -31.305 33.054 1.00 0.00 3A7 ATOM 2466 O VAL 350 6.691 -30.900 31.980 1.00 0.00 3A7 ATOM 2467 N LEU 351 6.619 -32.397 33.667 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2469 CB LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 4.203 -32.710 33.432 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00	ATOM	2463	CG1	VAL	350	9.700	-31.257	31.710	1.00	0.00	3A7
ATOM 2465 C VAL 350 7.128 -31.305 33.054 1.00 0.00 3A7 ATOM 2466 O VAL 350 6.691 -30.900 31.980 1.00 0.00 3A7 ATOM 2467 N LEU 351 6.619 -32.397 33.667 1.00 0.00 3A7 ATOM 2468 CA LEU 351 5.583 -33.220 33.098 1.00 0.00 3A7 ATOM 2469 CB LEU 351 5.689 -34.682 33.599 1.00 0.00 3A7 ATOM 2470 CG LEU 351 7.076 -35.324 33.599 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.162 -36.712 34.024 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 4.203 -32.710 33.432 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00											
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ATOM 2470 CG LEU 351 7.076 -35.324 33.359 1.00 0.00 3A7 ATOM 2471 CD1 LEU 351 7.162 -36.712 34.024 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 4.203 -32.710 33.432 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00 3A7	MOTA	2469	CB	LEU	351	5.689	-34.682	33.599	1.00	0.00	3A7
ATOM 2471 CD1 LEU 351 7.162 -36.712 34.024 1.00 0.00 3A7 ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A7 ATOM 2473 C LEU 351 4.203 -32.710 33.432 1.00 0.00 3A7 ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A7 ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00 3A7			CG			7.076	-35.324	33.359	1.00	0.00	3A7
ATOM 2472 CD2 LEU 351 7.441 -35.402 31.865 1.00 0.00 3A ⁻ ATOM 2473 C LEU 351 4.203 -32.710 33.432 1.00 0.00 3A ⁻ ATOM 2474 O LEU 351 3.248 -32.996 32.716 1.00 0.00 3A ⁻ ATOM 2475 N GLN 352 4.059 -31.949 34.546 1.00 0.00 3A ⁻											3A7
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ATOM 2475 N GLN 352 4.059 -31,949 34.546 1.00 0.00 3A											
ATOM 2476 CA GLN 352 2.775 -31.491 35.037 1.00 0.00 3A											3A7
	ATOM	2476	CA	GLN	352	2.775	-31.491	35.037	1.00	0.00	3A7

ATOM	2477	СВ	GLN	352	2.625	-31.677	36.565	1.00	0.00	3A7
ATOM	2478	CG	GLN	352		-33.072	36.977	1.00	0.00	3A7
ATOM	2479	CD	GLN	352		-34.176	36.678	1.00	0.00	3A7
ATOM	2480		GLN	352		-34.938	35.716	1.00	0.00	3A7
ATOM	2481		GLN	352		-34.268	37.551	1.00	0.00	3A7
ATOM	2482	С	GLN	352		-30.043	34.711	1.00	0.00	3A7
ATOM	2483	0	GLN	352		-29.394	35.333	1.00	0.00	3A7
ATOM	2484	N	LEU	353		-29.494	33.712	1.00	0.00	3A7
ATOM	2485	CA	LEU	353		-28.104	33.338	1.00	0.00	3A7
ATOM	2486	CB	LEU	353		-27.396	33.371	1.00	0.00	3A7
ATOM	2487	CG	LEU	353		-27.076	34.789	1.00	0.00	3A7
ATOM	2488		LEU	353		-26.787	34.712	1.00	0.00	3A7
ATOM	2489		LEU	353		-25.911	35.433	1.00	0.00	3A7
ATOM	2490	c	LEU	353		-28.000	31.951	1.00	0.00	3A7
ATOM	2491	0	LEU	353		-27.396	31.071	1.00	0.00	3A7
ATOM	2492	N	GLU	354	1.380	-28.556	31.747	1.00	0.00	3A7
ATOM	2493	CA	GLU	354		-28.679	30.481	1.00	0.00	3A7
ATOM	2494	СВ	GLU	354		-29.284	30.692	1.00	0.00	3A7
MOTA	2495	CG	GLU	354		-30.790	31.013	1.00	0.00	3A7
MOTA	2496	CD	GLU	354		-31.081	32.431	1.00	0.00	3A7
ATOM	2497		GLU	354		-31.962	32.579	1.00	0.00	3A7
MOTA	2498		GLU	354		-30.446	33.382	1.00	0.00	3A7
MOTA	2499	С	GLU	354		-27.384	29.710	1.00	0.00	3A7
ATOM	2500	0	GLU	354		-27.315	28.531	1.00	0.00	3A7
ATOM	2501	N	TYR	355	0.017	-26.319	30.358	1.00	0.00	3A7
MOTA	2502	CA	TYR	355		-25.056	29.708	1.00	0.00	3A7
ATOM	2503	СВ	TYR	355		-24.126	30.584	1.00	0.00	3A7
ATOM	2504	CG	TYR	355		-24.797	30.922	1.00	0.00	3A7
MOTA	2505	CD1	TYR	355	-2.853	-24.843	32.245	1.00	0.00	3A7
ATOM	2506	CD2	TYR	355	-3.183	-25.427	29.938	1.00	0.00	3A7
ATOM	2507	CE1	TYR	355	-4.029	-25.504	32.585	1.00	0.00	3A7
MOTA	2508	CE2	TYR	355	-4.354	-26.101	30.275	1.00	0.00	3A7
ATOM	2509	CZ	TYR	355	-4.779	-26.138	31.599	1.00	0.00	3A7
MOTA	2510	OH	TYR	355	-5.972	-26.813	31.940	1.00	0.00	3A7
ATOM	2511	С	TYR	355	1.014	-24.314	29.358	1.00	0.00	3A7
MOTA	2512	0	TYR	355	1.093	-23.672	28.320	1.00	0.00	3A7
ATOM	2513	N	LEU	356	2.069	-24.432	30.194	1.00	0.00	3A7
ATOM	2514	CA	LEU	356	3.372	-23.853	29.929	1.00	0.00	3A7
ATOM	2515	СВ	LEU	356		-24.000	31.136	1.00	0.00	3A7
ATOM	2516	CG	LEU	356		-22.859	31.211	1.00	0.00	3A7
ATOM	2517		reu	356		-22.429	32.674	1.00	0.00	3A7
ATOM	2518		LEU	356		-23.187	30.588	1.00	0.00	3A7
ATOM	2519	С	LEU	356		-24.430	28.735	1.00	0.00	3A7
ATOM	2520	0	LEU	356		-23.709	27.891	1.00	0.00	3A7
ATOM	2521	N	ASP	357		~25.778	28.619	1.00	0.00	3A7
ATOM	2522	CA	ASP	357		-26.516	27.513	1.00	0.00	3A7
ATOM	2523	CB	ASP	357		-28.050	27.598	1.00	0.00	3A7
ATOM ATOM	2524	CG	ASP	357		-28.771	28.597	1.00	0.00	3A7
ATOM	.2525 2526		ASP ASP	357	•	-29.726	28.159	1.00	0.00	3A7
ATOM	2527	C	ASP	357 357		-28.397 -26.136	29.796	1.00	0.00	3A7 3A7
ATOM	2528	Ö	ASP	357		-25.985	26.182 25.183	1.00	0.00	3A7
ATOM	2529	N	MET	358		-25.956	26.163	1.00	0.00	3A7
ATOM	2530	CA	MET	358		-25.573	24.997	1.00	0.00	3A7
ATOM	2531	СВ	MET	358		-25.711	25.263	1.00	0.00	3A7
ATOM	2532	CG	MET	358		-27.178	25.203	1.00	0.00	3A7
ATOM	2533	SD	MET	358		-27.420	26.341	1.00	0.00	3A7
ATOM	2534	CE	MET	358		-26.461	25.262	1.00	0.00	3A7
ATOM	2535	Č	MET	358		-24.149	24.601	1.00	0.00	3A7
ATOM	2536	ŏ	MET	358		-23.825	23.421	1.00	0.00	3A7
ATOM	2537	N	VAL	359		-23.255	25.594	1.00	0.00	3A7
ATOM	2538	CA	VAL	359		-21.869	25.376	1.00	0.00	3A7
ATOM	2539	СВ	VAL	359		-21.083	26.684	1.00	0.00	3A7
ATOM	2540		VAL	359		-19.776	26.626	1.00	0.00	3A7
ATOM	2541		VAL	359		-20.783	27.005	1.00	0.00	3A7
ATOM	2542	c	VAL	359		-21.791	24.701	1.00	0.00	3A7
ATOM	2543	ō	VAL	359		-21.063	23.725	1.00	0.00	3A7
ATOM	2544	N	VAL	360		-22.575	25.182	1.00	0.00	3A7
MOTA	2545	CA	VAL	360		-22.600	24.616	1.00	0.00	3A7
MOTA	2546	СВ	VAL	360		-23.421	25.479	1.00	0.00	3A7
ATOM	2547	CG1	VAL	360		-23.573	24.831	1.00	0.00	3A7
ATOM	2548	CG2	VAL	360	7.633	-22.713	26.844	1.00	0.00	3A7

ATOM 2549 C VAL 360 6.520 -23.153 23.207 1.00 0.00 3A7 7.168 -22.609 5.711 -24.208 1.00 0.00 3A7 ATOM 2550 ٥ VAL 360 22,323 ASN 1.00 0.00 3A7 ATOM 2551 N 361 22,949 MOTA 2552 CA ASN 361 5.556 -24.789 21.630 1.00 0.00 3A7 4.650 -26.030 21.669 1.00 0.00 ATOM 2553 CB ASN 361 3A7 MOTA 2554 CG ASN 361 5.417 -27.219 22.258 1.00 0.00 3A7 1.00 0.00 MOTA OD1 ASN 361 6.641 -27.329 22,121 3A7 2555 4.654 -28.135 ATOM 2556 ND2 ASN 361 22,930 1.00 0.00 3A7 2557 4.952 -23.808 20.655 1.00 0.00 MOTA С ASN 361 3A7 ATOM 2558 0 ASN 361 5.410 -23.694 19.523 1.00 0.00 3A7 3.925 -23.044 1.00 0.00 2559 GLU 362 21.087 3A7 ATOM N 3.338 -21.994 20.287 1.00 0.00 MOTA 2560 CA GLU 362 3A7 ATOM 2561 СВ GLU 362 2.013 -21.499 20.896 1.00 0.00 3A7 ATOM 2562 CG GLU 362 1.224 -20.515 20.011 1.00 0.00 3A7 2563 0.583 -21.183 18.798 1.00 0.00 3A7 MOTA CD GLU 362 0.987 -22.314 1.00 0.00 2564 OE1 GLU 18.429 3A7 ATOM 362 ATOM 2565 OE2 GLU 362 -0.309 -20.534 18.190 1.00 0.00 3A7 2566 4.241 -20.837 20.000 1.00 0.00 **3A7** ATOM C GLU 362 4.205 -20.266 MOTA 2567 362 18.913 1.00 0.00 3A7 0 GLU 0.00 5.135 -20.478 20.946 1.00 3A7 ATOM 2568 N THR 363 ATOM 2569 CA THR 363 6.090 -19.416 20.720 1.00 0.00 3A7 ATOM 2570 6.793 -19.002 21.991 1.00 0.00 3A7 CB THR 363 ATOM 2571 OG1 THR 363 5.804 -18.623 22.938 1.00 0.00 3A7 2572 7.691 -17.778 21.706 1.00 0.00 3A7 ATOM CG2 THR 363 7.091 -19.831 19.666 1.00 0.00 3A7 ATOM 2573 C THR 363 7.464 -19.042 ATOM 2574 0 THR 363 18.805 1.00 0.00 3A7 2575 7.504 -21.115 19.676 1.00 0.00 3A7 ATOM N LEU 364 8.417 -21.641 MOTA 2576 CA LEU 364 18.695 1.00 0.00 3A7 8.957 -23.014 19.086 1.00 0.00 3A7 **ATOM** 2577 CB LEU 364 0.00 ATOM 2578 CG LEU 364 9.921 -23.018 20.283 1.00 3A7 10.242 -24.462 MOTA 2579 CD1 LEU 364 20.696 1.00 0.00 3A7 ATOM 2580 CD2 LEU 364 11.219 -22.259 19.974 1.00 0.00 3A7 MOTA 2581 7.769 -21.746 17.338 1.00 0.00 3A7 LEU 364 С 8.410 -21.492 0.00 3A7 ATOM 2582 O 364 16.324 1.00 LEU 0.00 6.467 -22.094 **ATOM** 2583 N ARG 365 17.264 1.00 3A7 MOTA 2584 CA ARG 365 5.743 -22.109 16,003 1.00 0.00 3A7 4.300 -22.612 0.00 ATOM 2585 СВ ARG 365 16.169 1.00 3A7 MOTA 2586 3.614 -22.980 14.858 1.00 0.00 3A7 CG ARG 365 2.117 -23.285 15.005 0.00 ATOM 2587 CD ARG 365 1.00 3A7 ATOM 2588 NE ARG 365 1.371 -21.987 15.068 1.00 0.00 3A7 0.011 -21.942 **ATOM** 2589 CZ ARG 365 15.201 1.00 0.00 3A7 -0.637 -20.742 0.00 ATOM 2590 NH1 ARG 365 15.124 1.00 3A7 **ATOM** 2591 NH2 ARG -0.703 -23.084 15.418 1.00 0.00 3A7 365 ATOM 2592 5.648 -20.756 15.371 1.00 0.00 3A7 C ARG 365 **ATOM** 2593 O ΛRG 365 5.941 -20.573 14.192 1.00 0.00 3A7 ATOM 2594 LEU 366 5.239 -19.760 16.176 1.00 0.00 3A7 N ATOM 2595 CA LEU 366 5.030 -18.410 15.729 1.00 0.00 3A7 ATOM 2596 СВ LEU 366 4.204 -17.608 16.752 1.00 0.00 3A7 3.017 -16.833 2597 16.122 1.00 0.00 3A7 ATOM CG LEU 366 MOTA 2598 CD1 LEU 366 2.029 -16.361 17.201 1.00 0.00 3A7 MOTA 2599 LEU 3.452 -15.648 15.240 0.00 3A7 CD2 366 1.00 **ATOM** 2600 LEU 366 6.295 -17.670 15.380 1.00 0.00 3A7 С 6.339 -16.992 ATOM 2601 14.359 1.00 0.00 3A7 0 LEU 366 7.367 -17.798 ATOM 2602 N PHE 367 16.193 1.00 0.00 3A7 ATOM 2603 CA PHE 367 8.619 -17.136 15.897 1.00 0.00 3A7 ATOM 2604 8.999 -16.072 16.907 0.00 3A7 CB PHE 367 1.00 7.886 -15.081 ATOM 2605 CG PHE 367 17.042 1.00 0.00 3A7 6.921 -15.250 ATOM 2606 CD1 PHE 367 18,035 1.00 0.00 3A7 7.781 -13.998 ATOM 2607 CD2 PHE 367 16.170 1.00 0.00 3A7 MOTA 2608 CE1 PHE 367 5.855 -14.365 18.137 1.00 0.00 3A7 ATOM 2609 6.723 -13.100 0.00 3A7 CE2 PHE 367 16.285 1.00 ATOM 2610 PHE 5.757 -13.284 17.269 1.00 0.00 3A7 CZ 367 9.740 -18.121 ATOM 2611 С PHE 15.878 1.00 0.00 3A7 367 10.525 -18.207 3A7 ATOM 2612 0 PHE 367 16.823 1.00 0.00 ATOM 2613 PRO 368 9.897 -18.877 14.814 1.00 0.00 3A7 Ν MOTA 10.926 -19.868 0.00 3A7 2614 CA PRO 368 14.730 1.00 8.891 -19.039 ATOM 2615 CD PRO 368 13.788 1.00 0.00 3A7 ATOM 10.570 -20.710 13.544 1.00 0.00 3A7 2616 CB PRO 368 9.531 -19.942 ATOM 2617 CG PRO 368 12.757 1.00 0.00 3A7 MOTA 2618 С PRO 368 12.257 -19.200 14.589 1.00 0.00 3A7 MOTA 2619 0 PRO 368 12.479 -18.434 13.657 1.00 0.00 3A7 MOTA 2620 13.143 -19.481 1.00 0.00 3A7 N VAL 369 15.561

ATOM	2621	CA	VAL	369	14.427 -	18.858	15.709	1.00	0.00	3A7
ATOM	2622	СВ	VAL	369	15.058 -		16.991	1.00	0.00	3A7
								1.00		3A7
ATOM	2623	CG1		369	16.449 -		17.115		0.00	
MOTA	2624	CG2	VAL	369	14.135 -		18.133	1.00	0.00	3A7
ATOM	2625	С	VAL	369	15.330 -	19.141	14.529	1.00	0.00	3A7
ATOM	2626	0	VAL	369	16.105 -		14.109	1.00	0.00	3A7
	2627		ALA	370	15.232 -		13.946	1.00	0.00	3A7
ATOM		N								
ATOM	2628	CA	ALA	370	15.984 -		12.775	1.00	0.00	3A7
ATOM	2629	CB	ALA	370	16.677 -	-22.035	12.966	1.00	0.00	3A7
ATOM	2630	С	ALA	370	15.038 -	-20.739	11.619	1.00	0.00	3A7
ATOM	2631	ō	ALA	370	14.503 -		11.309	1.00	0.00	3A7
										3A7
ATOM	2632	N	MET	371	14.813 -		10.938	1.00	0.00	
ATOM	2633	CA	MET	371	13.787 -	-19.436	9.924	1.00	0.00	3A7
ATOM	2634	CB	MET	371	13.599 -	-17.940	9.616	1.00	0.00	3A7
ATOM	2635	CG	MET	371	14.852 -	-17.053	9.800	1.00	0.00	3A7
		SD	MET	371	16.175 -		8.566	1.00	0.00	3A7
ATOM	2636									
ATOM	2637	CE	MET	371	15.303 -		7.182	1.00	0.00	3A7
ATOM	2638	С	MET	371	14.093	-20.142	8.625	1.00	0.00	3A7
ATOM	2639	0	MET	371	13.208 -	-20.260	7.783	1.00	0.00	3A7
ATOM	2640	N	ARG	372	15.346 -	-20 621	8.432	1.00	0.00	3A7
							7.254	1.00	0.00	3A7
ATOM	2641	CA	ARG	372	15.716					
MOTA	2642	СВ	ARG	372	16.208 -	-20.480	6.088	1.00	0.00	3A7
ATOM	2643	CG	ARG	372	15.140 -	-19.769	5.248	1.00	0.00	3A7
ATOM	2644	CD	ARG	372	15.828	-19.020	4.096	1.00	0.00	3A7
ATOM	2645	NE	ARG	372	14.871		2.996	1.00	0.00	3A7
MOTA	2646	CZ	ARG	372	14.486		2.066	1.00	0.00	3A7
MOTA	2647	NH1	ARG	372	13.971 -	~19.194	0.870	1.00	0.00	3A7
MOTA	2648	NH2	ARG	372	14.646	-20.930	2.301	1.00	0.00	3A7
ATOM	2649	С	ARG	372	16.832	-22.309	7.639	1.00	0.00	3A7
			ARG	372	17.619		8.542	1.00	0.00	3A7
ATOM	2650	0								
ATOM	2651	N	ren	373	16.916		6.907	1.00	0.00	3A7
ATOM	2652	CA	LEU	373	17.947	-24.462	7.034	1.00	0.00	3A7
MOTA	2653	ÇВ	LEU	373	17.400	-25.879	7.360	1.00	0.00	3A7
ATOM	2654	CG	LEU	373	16.633		8.700	1.00	0.00	3A7
									0.00	3A7
ATOM	2655		LEU	373	17.347		9.860	1.00		
ATOM	2656	CD2	LEU	373	15.150	-25.605	8.611	1.00	0.00	3A7
MOTA	2657	С	LEU	373	18.641	-24.532	5.697	1.00	0.00	3A7
ATOM	2658	0	LEU	373	18.145	-23.979	4.717	1.00	0.00	3A7
ATOM	2659	N	GLU	374	19.806		5.619	1.00	0.00	3A7
										3A7
ATOM	2660	CA	GLU	374	20.496		4.356	1.00	0.00	
ATOM	2661	CB	GLU	374	21.788	-24.637	4.153	1.00	0.00	3A7
ATOM	2662	CG	GLU	374	21.575	-23.121	4.279	1.00	0.00	3A7
ATOM	2663	CD	GLU	374	22.909		4.038	1.00	0.00	3A7
ATOM	2664		GLU	374	23.435		5.000	1.00	0.00	3A7
ATOM	2665		GLU	374	23.420		2.889	1.00	0.00	3A7
ATOM	2666	С	GLU	374	20.862	-26.936	4.222	1.00	0.00	3 A 7
ATOM	2667	0	GLU	374	21.393	-27.553	5.141	1.00	0.00	3A7
ATOM	2668	N	ARG	375	20.591	-27.510	3.026	1.00	0.00	3A7
ATOM	2669	CA	ARG	375		-28.878	2.666	1.00	0.00	3A7
				-						3A7
MOTA	2670	СВ	ARG	375		-29.770	2.636	1.00	0.00	
MOTA	2671	CG	ARG	375		-30.018	4.037	1.00	0.00	3A7
ATOM	2672	CD	ARG	• 375	17.789	-30.919	4.035	1.00	0.00	3A7
ATOM	2673	NE	ARG	375	17.499	-31.381	5.436	1.00	0.00	3A7
ATOM	2674	cz	ARG	375		-30.590	6.396	1.00	0.00	3A7
									0.00	3A7
ATOM	2675		ARG	375		-31.096	7.650	1.00		
ATOM	2676	NH2	ARG	375		-29.307	6.125	1.00	0.00	3A7
ATOM	2677	С	ARG	375	21.494	-28.826	1.293	1.00	0.00	3A7
ATOM	2678	0	ARG	375	21.347	-27.846	0.569	1.00	0.00	3A7
ATOM	2679	N	VAL	376		-29.890	0.889		0.00	3A7
										3A7
ATOM	2680	CA	VAL	376		-29.949	-0.420	1.00	0.00	
ATOM	2681	CB	VAL	376		-29.725	-0.397		0.00	3A7
MOTA	2682	CG1	VAL	376	24.936	-29.796	-1.822	1.00	0.00	3A7
ATOM	2683		VAL	376	24.638	-28.346	0.234	1.00	0.00	3A7
ATOM	2684	c	VAL	376		-31.316	-0.934		0.00	3A7
										3A7
ATOM	2685	0	VAL	376		-32.316	-0.233		0.00	
ATOM	2686	Ŋ	CYS	377		-31.397	-2.212		0.00	3A7
MOTA	2687	CA	CYS	377	21.721	-32.642	-2.851	1.00	0.00	3A7
MOTA	2688	СВ	CYS	377	20.821	-32.435	-4.083	1.00	0.00	3A7
ATOM	2689	SG	CYS	377		-31.876	-3.569		0.00	3A7
						-33.392			0.00	3A7
ATOM	2690	C	CYS	377			-3.254			
ATOM	2691	0	CYS	377		-32.843	-3.794		0.00	3A7
ATOM	2692	N	LYS	378	22.964	-34.705	-2.955	1.00	0.00	3A7

MOTA	2693	CA	LYS	378	24.083 -35.594 -3.143 1.00 0.00	3A7
MOTA	2694	СВ	LYS	378	24.073 -36.718 -2.075 1.00 0.00	3A7
ATOM	2695	CG	LYS	378	23.127 -36.428 -0.894 1.00 0.00	3A7
MOTA	2696	CD	LYS	378	23.024 -37.592 0.101 1.00 0.00	3A7
MOTA	2697	CE	LYS	378	21.948 -37.375 1.174 1.00 0.00	3A7
MOTA	2698	NZ	LYS	378	22.223 -36.159 1.974 1.00 0.00	3A7
MOTA	2699	С	LYS	378	24.040 -36.202 -4.524 1.00 0.00	3A7
MOTA	2700	0	LYS	378	25.062 -36.609 -5.075 1.00 0.00	3A7
ATOM	2701	N	LYS	379	22.814 -36.285 -5.081 1.00 0.00	3A7
ATOM	2702	CA	LYS	379	22.547 -36.939 -6.329 1.00 0.00	3A7
ATOM	2703	CB	LYS	379	22.121 -38.417 -6.127 1.00 0.00 20.935 -38.609 -5.161 1.00 0.00	3A7 3A7
ATOM ATOM	2704 2705	CG CD	LYS LYS	379 379	20.935 -38.609 -5.161 1.00 0.00 20.582 -40.083 -4.899 1.00 0.00	3A7
ATOM	2706	CE	LYS	379	21.665 -40.842 -4.120 1.00 0.00	3A7
ATOM	2707	NZ	LYS	379	21.236 -42.233 -3.850 1.00 0.00	3A7
ATOM	2708	c	LYS	379	21.450 -36.155 -6.981 1.00 0.00	3A7
ATOM	2709	0	LYS	379	21.014 -35.119 -6.483 1.00 0.00	3A7
ATOM	2710	N	ASP	380	20.951 -36.650 -8.134 1.00 0.00	3A7
ATOM	2711	CA	ASP	380	19.820 -36.071 -8.818 1.00 0.00	3A7
ATOM	2712	CB	ASP	380	19.811 -36.404 -10.323 1.00 0.00	3A7
ATOM	2713	CG	ASP	380	21.092 -35.921 -10.999 1.00 0.00	3A7
ATOM	2714		ASP	380	21.347 -34.689 -10.981 1.00 0.00	3A7
ATOM	2715		ASP	380	21.824 -36.782 -11.556 1.00 0.00	3A7
ATOM	2716	C	ASP	380	18.562 -36.616 -8.182 1.00 0.00	3A7
ATOM	2717	0	ASP	380	18.496 -37.798 -7.848 1.00 0.00	3A7 3A7
ATOM ATOM	2718 2719	N CA	VAL VAL	381 381	17.554 -35.744 -7.966 1.00 0.00 16.378 -36.118 -7.224 1.00 0.00	3A7
ATOM	2720	CB	VAL	381	16.557 -35.910 -5.720 1.00 0.00	3A7
ATOM	2721		VAL	381	16.853 -34.439 -5.360 1.00 0.00	3A7
ATOM	2722		VAL	381	15.353 -36.489 -4.947 1.00 0.00	3A7
ATOM	2723	С	VAL	381	15.248 -35.308 -7.781 1.00 0.00	3A7
MOTA	2724	0	VAL	381	15.417 -34.151 -8.142 1.00 0.00	3A7
MOTA	2725	N	GLU	382	14.045 -35.908 -7.874 1.00 0.00	3A7
MOTA	2726	CA	GLU	382	12.888 -35.247 -8.420 1.00 0.00	3A7
ATOM ATOM	2727 2728	CB CG	GLU GLU	382 382	12.165 -36.100 -9.485 1.00 0.00 12.963 -36.325 -10.781 1.00 0.00	3A7 3A7
ATOM	2729	CD	GLU	382	14.109 -37.311 -10.571 1.00 0.00	3A7
ATOM	2730		GLU	382	13.827 -38.470 -10.163 1.00 0.00	3A7
ATOM	2731		GLU	382	15.281 -36.921 -10.822 1.00 0.00	3A7
MOTA	2732	С	GLU	382	11.952 -34.980 -7.271 1.00 0.00	3A7
ATOM	2733	0	GLU	382	11.531 -35.909 -6.587 1.00 0.00	3A7
ATOM	2734	N	ILE	383	11.615 -33.690 -7.028 1.00 0.00	3A7
ATOM	2735	CA	ILE	383	10.762 -33.270 -5.937 1.00 0.00	3A7
ATOM	2736 2737	CB	ILE	383 383	11.449 -32.299 -4.973 1.00 0.00 10.543 -32.043 -3.747 1.00 0.00	3A7 3A7
ATOM ATOM	2738		ILE	383	12.865 -32.774 -4.555 1.00 0.00	3A7
ATOM	2739	CD	ILE	383	12.883 -34.026 -3.677 1.00 0.00	3A7
ATOM	2740	c	ILE	383	9.578 -32.594 -6.567 1.00 0.00	3A7
ATOM	2741	Ο.	ILE	383	9.686 -31.493 -7.103 1.00 0.00	. 3A7
ATOM	2742	N	ASN	384	8.399 -33.254 -6.521 1.00 0.00	3A7
ATOM	2743	CA	ASN	384	7.130 -32.719 -6.976 1.00 0.00	3A7
ATOM	2744	CB	ASN	384	6.732 -31.411 -6.222 1.00 0.00	3A7
ATOM	2745 2746	CG	ASN	384	5.218 -31.147 -6.283 1.00 0.00 4.758 -30.251 -7.000 1.00 0.00	3A7 3A7
ATOM ATOM	2747		ASN ASN	384 384	4.443 -31.956 -5.498 1.00 0.00	3A7
ATOM	2748	c	ASN	384	7.100 -32.504 -8.480 1.00 0.00	3A7
ATOM	2749	ō	ASN	384	6.410 -31.623 -8.988 1.00 0.00	3A7
ATOM	2750	N	GLY	385	7.870 -33.322 -9.231 1.00 0.00	3A7
ATOM	2751	CA	GLY	385	7.911 -33.246 -10.666 1.00 0.00	3A7
ATOM	2752	С	GLY	385	9.013 -32.342 -11.156 1.00 0.00	3A7
ATOM	2753	0	GLY	385	9.217 -32.266 -12.366 1.00 0.00	3A7
ATOM	2754	N	MET	386	9.762 -31.631 -10.264 1.00 0.00	3A7
ATOM ATOM	2755 2756	CA CB	MET MET	386 386	10.855 -30.773 -10.695 1.00 0.00 10.660 -29.264 -10.426 1.00 0.00	3A7 3A7
ATOM	2757	CG	MET	386	10.337 -28.845 -8.990 1.00 0.00	3A7
ATOM	2758	SD	MET	386	9.854 -27.091 -8.895 1.00 0.00	3A7
ATOM	2759	CE	MET	386	11.448 -26.373 -9.388 1.00 0.00	3A7
ATOM	2760	C	MET	386	12.159 -31.305 -10.187 1.00 0.00	3A7
MOTA	2761	0	MET	386	12.335 -31.654 -9.025 1.00 0.00	3A7
ATOM	2762	N	PHE	387	13.122 -31.396 -11.125 1.00 0.00	3A7
ATOM	2763	CA	PHE	387	14.382 -32.074 -10.982 1.00 0.00	3A7
ATOM	2764	СВ	PHE	387	14.935 -32.474 -12.378 1.00 0.00	3A7

ATOM	2765	CG	PHE	387	14.102 -	-33.505	-13.091	1.00	0.00	3A7
ATOM	2766	CD1	PHE	387	14.645 -	-34.767	-13.344	1.00	0.00	3A7
ATOM	2767	CD2		387	12.827 -	-33.213	-13.585	1.00	0.00	3A7
ATOM	2768	CE1		387	13.920			1.00	0.00	3A7
					12.097 -			1.00	0.00	3A7
ATOM	2769	CE2		387						
ATOM	2770	CZ	PHE	387	12.642			1.00	0.00	3A7
ATOM	2771	С	PHE	387	15.405 -			1.00	0.00	3A7
ATOM	2772	0	PHE	387	15.631 -	-30.043	-10.726	1.00	0.00	3A7
ATOM	2773	N	ILE	388	16.066	-31.706	-9.251	1.00	0.00	3A7
ATOM	2774	ÇA	ILE	388	17.145		-8.544	1.00	0.00	3A7
					16.994		-7.032	1.00	0.00	3A7
ATOM	2775	CB	ILE	388						
ATOM	2776	CG2		388	18.144		-6.387	1.00	0.00	3A7
MOTA	2777	CG1	ILE	388	15.641	-30.487	-6.591	1.00	0.00	3A7
ATOM	2778	CD	ILE	388	15.434	-29.010	-6.913	1.00	0.00	3A7
ATOM	2779	С	ILE	388	18.438	-31.746	-8.935	1.00	0.00	3A7
ATOM	2780	0	ILE	388	18.576	-32.952	-8.728	1.00	0.00	3A7
ATOM	2781	N	PRO	389	19.415		-9.496	1.00	0.00	3A7
							-9.867	1.00	0.00	3A7
MOTA	2782	CA	PRO	389	20.698					
MOTA	2783	CD	PRO	389		-29.901		1.00	0.00	3A7
MOTA	2784	ÇВ	PRO	389	21.290	-30.549	-10.822	1.00	0.00	3A7
MOTA	2785	CG	PRO	389	20.081	-29.931	-11.509	1.00	0.00	3A7
ATOM	2786	С	PRO	389	21.614	-31.785	-8.684	1.00	0.00	3A7
ATOM	2787	ō	PRO	389	21.474		-7.659	1.00	0.00	3A7
					22.627		-8.836	1.00	0.00	3A7
ATOM	2788	N	LYS	390						
ATOM	2789	CA	LY\$	390	23.654		-7.847	1.00	0.00	3A7
MOTA	2790	CB	LYS	390	24.733	-33.851	-8.363	1.00	0.00	3A7
ATOM	2791	CG	LYS	390	24.234	-35.053	-9.176	1.00	0.00	3A7
ATOM	2792	CD	LY\$	390	25.372	-36.029	-9.517	1.00	0.00	3A7
ATOM	2793	CE	LYS	390	24.921	-37.258	-10.316	1.00	0.00	3A7
ATOM	2794	NZ	LYS	390	23.959		-9.538	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	2795	C	LYS	390	24.346		-7.486			
ATOM	2796	0	LYS	390		-30.776	-8.366	1.00	0.00	3A7
ATOM	2797	N	GLY	391	24.558	-31.329	-6.177	1.00	0.00	3A7
ATOM	2798	CA	GLY	391	25.250	-30.153	-5.707	1.00	0.00	3A7
MOTA	2799	С	GLY	391	24.397	-28.926	-5.567	1.00	0.00	3A7
ATOM	2800	ō	GLY	391		-27.848	-5.320	1.00	0.00	3A7
ATOM	2801	N	VAL	392		-29.029	-5.690	1.00	0.00	3A7
						-27.896	-5.522	1.00	0.00	3A7
ATOM	2802	CA	VAL	392						
ATOM	2803	CB	VAL	392		-28.126	-6.224	1.00	0.00	3A7
ATOM	2804	CG1	VAL	392	19.765	-27.062	-5.883	1.00	0.00	3A7
ATOM	2805	CG2	VAL	392	21.074	-28.134	-7.744	1.00	0.00	3A7
MOTA	2806	С	VAL	392	21.922	-27.684	-4.050	1.00	0.00	3A7
ATOM	2807	Ō	VAL	392		-28.644	-3.290	1.00	0.00	3A7
ATOM	2808	N	VAL	393		-26.403	-3.629	1.00	0.00	3A7
									0.00	3A7
ATOM	2809	CA	VAL	393		-26.024	-2.268	1.00		
ATOM	2810	CB	VAL	393		-24.695		1.00	0.00	3A7
ATOM	2811	CG1	VAL	393	21.828	-24.336	-0.425	1.00	0.00	3A7
ATOM	2812	CG2	VAL	393	23.636	-24.785	~2.160	1.00	0.00	3A7
ATOM	2813	С	VAL	393	19.992	-25.964	-2.130	1.00	0.00	3A7
ATOM	2814	ō	VAL	393		-25.288		1.00	0.00	3A7
ATOM	2815	N	VAL	394		-26.712		1.00	0.00	3A7
									0.00	3A7
MOTA	2816	CA	VAL	394		-26.825		1.00		
MOTA	2817	СВ	VAL	394		-28.282		1.00	0.00	3A7
ATOM	2818	CG1	VAL	394	16.104	-28.411	-0.510	1.00	0.00	3 A7
ATOM	2819	CG2	VAL	394	17.948	-28.936	-2.163	1.00	0.00	3A7
ATOM	2820	С	VAL	394	17.840	-26.177	0.471	1.00	0.00	3A7
ATOM	2821	ō	VAL	394		-26.423		1.00	0.00	3A7
						-25.325		1.00	0.00	3A7
ATOM	2822	N	MET	395						3A7
MOTA	2823	CA	MET	395		-24.656		1.00	0.00	
ATOM	2824	СВ	MET	395	. 16.818	-23.145		1.00	0.00	3A7
ATOM	2825	CG	MET	395	18.304	-22.812	1.578	1.00	0.00	3A7
ATOM	2826	SD	MET	395	18.747	-21.101	2.015	1.00	0.00	3A7
ATOM	2827	CE	MET	395		-20.277		1.00	0.00	3A7
ATOM	2828	C	MET	395		-24.885		1.00	0.00	3A7
									0.00	3A7
ATOM	2829	0	MET	395		-24.925		1.00		
ATOM	2830	N	ILE	396		-25.076		1.00	0.00	3A7
MOTA	2831	CA	ILE	396	13.536	-25.356		1.00	0.00	3A7
ATOM	2832	CB	ILE	396	13.599	-26.610	4.904	1.00	0.00	3A7
ATOM	2833		ILE	396		-26.667		1.00	0.00	3A7
ATOM	2834		ILE	396		-27.897		1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	2835	CD	ILE	396		-28.104				
MOTA	2836	С	ILE	396	13.188	-24.182	4.902	1.00	0.00	3A7

ATOM	2837	0	ILE	396	13.874	-23.964	5.894	1.00	0.00	3A7
ATOM	2838	N	PRO	397	12.167	-23.398	4.590	1.00	0.00	3A7
MOTA	2839	CA	PRO	397	11.790		5.462	1.00	0.00	3A7
ATOM	2840	CD	PRO	397	11.961		3.209	1.00	0.00	3A7
ATOM	2841	СВ	PRO	397	11.201		4.533	1.00	0.00	3A7
ATOM	2842	CG	PRO	397	10.809		3.293	1.00	0.00	3A7
ATOM	2843	C	PRO PRO	397 397	10.834		6.544 6.310	1.00	0.00	3A7 3A7
ATOM ATOM	2844 2845	O N	SER	398	11.352	-22.732	7.767	1.00	0.00	3A7
ATOM	2846	CA	SER	398	10.575		8.914	1.00	0.00	3A7
ATOM	2847	СВ	SER	398		-23.676	10.138	1.00	0.00	3A7
ATOM	2848	ŌĞ	SER	398		-22.517	10.613	1.00	0.00	3A7
ATOM	2849	С	SER	398		-22.379	9.316	1.00	0.00	3A7
ATOM	2850	0	SER	398	8.422	-22.745	9.668	1.00	0.00	3A7
ATOM	2851	N	TYR	399		-21.053	9.231	1.00	0.00	3A7
ATOM	2852	CA	TYR	399		-19.958	9.507	1.00	0.00	3A7
ATOM	2853	CB	TYR	399		-18.562	9.264	1.00	0.00	3A7
ATOM	2854	CG	TYR	399		-17.492	10.212	1.00	0.00	3A7
ATOM	2855		TYR	399 399		-16.936	11.172	1.00 1.00	0.00	3A7 3A7
MOTA MOTA	2856 2857	CD2	TYR	399		-17.008 -15.959	10.123 12.051	1.00	0.00	3A7
ATOM	2858		TYR	399		-16.041	11.007	1.00	0.00	3A7
ATOM	2859	CZ	TYR	399		-15.520	11.975	1.00	0.00	3A7
ATOM	2860	ОН	TYR	399		-14.553	12.880	1.00	0.00	3A7
ATOM	2861	С	TYR	399		-20.038	8.647	1.00	0.00	3A7
ATOM	2862	0	TYR	399	6.567	-19.765	9.067	1.00	0.00	3A7
MOTA	2863	N	VAL	400	7.911	-20.472	7.398	1.00	0.00	3A7
ATOM	2864	CA	VAL	400		-20.616	6.436	1.00	0.00	3A7
MOTA	2865	СВ	VAL	400		-20.658	5.045	1.00	0.00	3A7
ATOM	2866		VAL	400		-20.758	4.020	1.00	0.00	3A7
ATOM ATOM	2867 2868	CGZ	VAL VAL	400 400		-19.308 -21.827	4.899 6.653	1.00	0.00	3A7 3A7
ATOM	2869	0	VAL	400		-21.734	6.547	1.00	0.00	3A7
ATOM	2870	N	LEU	401		-22.992	6.970	1.00	0.00	3A7
ATOM	2871	CA	LEU	401		-24.224	7.175	1.00	0.00	3A7
ATOM	2872	СВ	LEU	401		-25.449	7.318	1.00	0.00	3A7
ATOM	2873	CG	LEU	401	8.101	-25.453	6.535	1.00	0.00	3A7
MOTA	2874	CD1	LEU	401		-26.722	6.915	1.00	0.00	3A7
ATOM	2875		LEU	401		-25.294	5.023	1.00	0.00	3A7
MOTA	2876	C	LEU	401		-24.186	8.449	1.00	0.00	3A7
ATOM	2877	0	LEU	401		-24.705	8.504	1.00	0.00	3A7
ATOM ATOM .	2878 2879	N CA	HIS HIS	402 402		-23.512 -23.303	9.509 10.782	1.00	0.00	3A7 3A7
ATOM	2880		HIS	402		-24.809	12.042	1.00	0.00	3A7
ATOM	2881	CG	HIS	402		-23.553	12.480	1.00	0.00	3A7
ATOM	2882	СВ	HIS	402		-22.628	11.778	1.00	0.00	3A7
MOTA	2883	NE2	HIS	402	8.734	-24.122	13.375	1.00	0.00	3A7
MOTA	2884		HIS	402	7.762	-23.155	13.305	1.00	0.00	3A7
ATOM	2885		HIS	402	•	-25.085	12.595	1.00	0.00	3A7
ATOM	2886	С	HIS	402		-22.420	10.674	1.00	0.00	3A7
ATOM	2887	0	HIS	402		-22.343	11.602	1.00	0.00	3A7
ATOM ATOM	2888 2889	N CA	HIS HIS	403 403		-21.730 -20.839	9.522 9.280	1.00	0.00	3A7 3A7
ATOM	2890		HIS	403		~19.115	10.966	1.00	0.00	3A7
ATOM	2891	CG	HIS	403		-18.746	10.299	1.00	0.00	3A7
ATOM	2892	СВ	HIS	403		-19.394	9.048	1.00	0.00	3A7
ATOM	2893		HIS	403		-17.451	12.131	1.00	0.00	3A7
MOTA	2894	CD2	HIS	403	2.852	~17.730	11.028	1.00	0.00	3A7
MOTA	2895	CE1	HIS	403	4.638	-18.308	12.051	1.00	0.00	3A7
ATOM	2896	С	HIS	403		-21.280	8.096	1.00	0.00	3A7
MOTA	2897	0	HIS	403		-20.492	7.500	1.00	0.00	3A7
MOTA	2898	N	ASP	404		-22.588 -23.143	7.740	1.00	0.00	3A7
ATOM ATOM	2899 2900	CA CB	ASP	404 404		-23.143 -24.585	6.662 6.322	1.00	0.00	3A7 3A7
ATOM	2900	CG	ASP ASP	404		-24.585	5.103	1.00	0.00	3A7
ATOM	2902		ASP	404		-24.540	4.402	1.00	0.00	3A7
ATOM	2903		ASP	404		-26.417	4.850	1.00	0.00	3A7
ATOM	2904	C	ASP	404		-23.164	7.105	1.00	0.00	3A7
ATOM	2905	0	ASP	404		-23.809	8.108	1.00	0.00	3A7
MOTA	2906	N	PRO	405		-22.474	6.421	1.00	0.00	3A7
MOTA	2907	CA	PRO	405		-22.344	6.827	1.00	0.00	3A7
ATOM	2908	CD	PRO	405	-1.277	-21.674	5.237	1.00	0.00	3A7

ATOM	2909	СВ	PRO	405	~3.543	-21.309	5.854	1.00	0.00	3A7
MOTA	2910	CG	PRO	405	-2.641	-21.373	4.621	1.00	0.00	3A7
ATOM	2911	C	PRO	405	-3.739		6.756	1.00	0.00	3A7
ATOM	2912	ŏ	PRO	405	-4.766		7.420	1.00	0.00	3A7
ATOM	2913	N	LYS	406	-3.297		5.989	1.00	0.00	3A7
MOTA	2914	CA	LYS	406	-3.983		5.892	1.00	0.00	3A7
ATOM	2915	CB	LYS	406	-3.545	-26.748	4.646	1.00	0.00	3A7
ATOM	2916	CG	LYS	406	-3.805	-26.004	3.326	1.00	0.00	3 A 7
ATOM	2917	CD	LYS	406	-3.234	-26.692	2.072	1.00	0.00	3A7
ATOM	2918	CE	LYS	406	-3.939		1.650	1.00	0.00	3A7
									0.00	3A7
MOTA	2919	NZ	LYS	406	-3.601		2.541	1.00		
MOTA	2920	С	LYS	406	-3.730		7.115	1.00	0.00	3A7
MOTA	2921	0	LYS	406	-4.554		7.479	1.00	0.00	3A7
MOTA	2922	N	TYR	407	-2.572	-26.584	7.783	1.00	0.00	3A7
ATOM	2923	CA	TYR	407	-2.174	~27.340	8.948	1.00	0.00	3A7
MOTA	2924	СВ	TYR	407	-0.677	-27.703	8.898	1.00	0.00	3A7
MOTA	2925	CG	TYR	407	-0.579		8.000	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	2926		TYR	407	-0.674		6.613			
ATOM	2927		TYR	407	-0.492		8.557	1.00	0.00	3A7
ATOM	2928	CEl	TYR	407	-0.693	-29.912	5.799	1.00	0.00	3A7
ATOM	2929	CE2	TYR	407	-0.483	-31.314	7.746	1.00	0.00	3A7
ATOM	2930	CZ	TYR	407	-0.585	-31.179	6.365	1.00	0.00	3A7
ATOM	2931	ОН	TYR	407	-0.583		5.538	1.00	0.00	3A7
ATOM	2932	C	TYR	407	-2.474		10.218	1.00	0.00	3A7
							11.229	1.00	0.00	3A7
ATOM	2933	0	TYR	407	-2.827					
ATOM	2934	N	TRP	408	-2.334		10.202	1.00	0.00	3A7
ATOM	2935	CA	TRP	408	-2.553		11.368	1.00	0.00	3A7
MOTA	2936	СВ	TRP	408	-1.243	-23.786	11.891	1.00	0.00	3A7
ATOM	2937	CG	TRP	408	-0.242	-24.837	12.291	1.00	0.00	3A7
ATOM	2938	CD2	TRP	408	-0.524	-25.818	13.304	1.00	0.00	3A7
ATOM	2939		TRP	408		-25.107	11.823	1.00	0.00	3A7
ATOM	2940		TRP	408		-26.195	12.482	1.00	0.00	3A7
ATOM	2941		TRP	408		-26.677	13.353	1.00	0.00	3A7
ATOM	2942		TRP	408		-26.011	14.121	1.00	0.00	3A7
ATOM	2943	C22	TRP	408	0.578	-27.783	14.170	1.00	0.00	3A7
ATOM,	2944	CZ3	TRP	408	-1.597	-27.102	14.983	1.00	0.00	3A7
ATOM	2945	CH2	TRP	408	-0.524	-27.989	14.995	1.00	0.00	3A7
ATOM	2946	С	TRP	408		-23.347	10.974	1.00	0.00	3A7
ATOM	2947	ŏ	TRP	408		-22.324	10.383	1.00	0.00	3A7
									0.00	3A7
ATOM	2948	N	THR	409		-23.556	11.320	1.00		
ATOM	2949	CA	THR	409		-22.587	11.078	1.00	0.00	3A7
MOTA	2950	CB	THR	409		-23.197	11.275	1.00	0.00	3A7
ATOM	2951	OG1	THR	409	-8.322	-22.316	10.873	1.00	0.00	3A7
MOTA	2952	CG2	THR	409	-7.503	-23.671	12.727	1.00	0.00	3A7
ATOM	2953	С	THR	409	-5.686	-21.354	11.951	1.00	0.00	3A7
ATOM	2954	ŏ	THR	409		-21.439	13.116	1.00	0.00	3A7
ATOM	2955	N	GLU	410		-20.153	11.363	1.00	0.00	3A7
MOTA	2956	CA	GLU	410		-18.880	11.957	1.00	0.00	3A7
ATOM	2957	CB	GLU	. 410		-18.485	13.138	1.00	0.00	3A7
MOTA	2958	ÇG	GLU	410		-18.447	12.751	1.00	0.00	3A7
ATOM	2959	CD	GLU	410	-8.744	-18.043	13.970	1.00	0.00	3A7
MOTA	2960	OE1	GLU	410	-8.705	-18.790	14.985	1.00	0.00	3A7
ATOM	2961		GLU	410		-16.984	13.903	1.00	0.00	3A7
ATOM	2962	С	GLU	410		-18.872	12.399	1.00	0.00	3A7
ATOM	2963	ŏ	GLU	410		-18.654	13.572	1.00	0.00	3A7
ATOM	2964	N	PRO	411		-19.188	11.476	1.00	0.00	3A7
ATOM	2965	CA	PRO	411		-19.438	11.747	1.00	0.00	3A7
ATOM	2966	CD	PRO	411	-3.394	-19.045	10.041	1.00	0.00	3 A 7
ATOM	2967	CB	PRO	411	-1.144	-19.794	10.370	1.00	0.00	3A7
ATOM	2968	CG	PRO	411	-2.020	-19.039	9.368	1.00	0.00	3A7
ATOM	2969	c	PRO	411		-18.216	12.290	1.00	0.00	3A7
ATOM	2970	ŏ	PRO	411		-18.335	12.931	1.00	0.00	3A7
ATOM									0.00	3A7
	2971	N	GLU	412		-17.019	12.058	1.00		
ATOM	2972	CA	GLU	412		-15.791	12.493	1.00	0.00	3A7
ATOM	2973	CB	GLU	412		-14.650	11.516	1.00	0.00	3A7
MOTA	2974	CG	GLU	412	-0.914	-14.895	10.063	1.00	0.00	3A7
ATOM	2975	CD	GLU	412	0.609	-14.849	9.920	1.00	0.00	3A7
ATOM	2976		GLU	412		-15.190	8.807	1.00	0.00	3A7
ATOM	2977		GLU	412		-14.468	10.897	1.00	0.00	3A7
							13.903	1.00	0.00	3A7
ATOM	2978	C	GLU	412		-15.419				
ATOM	2979	0	GLU	412		-14.360	14.405	1.00	0.00	3A7
MOTA	2980	N	LYS	413	-2.226	-16.290	14.589	1.00	0.00	3A7

ATOM	2981	CA	LYS	413	-2.691 -	16.035	15.932	1.00	0.00	3A7
ATOM	2982	СВ	LYS	413	-4.204 -		16.093	1.00	0.00	3A7
ATOM	2983	CG	LYS	413	-5.059 -		15.276		0.00	3A7 3A7
ATOM	2984	CD	LYS	413	-6.569 -		15.519	1.00	0.00	3A7
ATOM	2985	CE	LYS	413	-7.012 -		16.938 17.084	1.00	0.00 0.00	3A7
MOTA	2986 2987	NZ	LYS	413	-8.477 - -1.939 -		16.917	1.00	0.00	3A7
ATOM ATOM	2988	С О	LYS LYS	413 413	-1.731 -		16.718	1.00	0.00	3A7
ATOM	2989	N	PHE	414	-1.550 -		18.059	1.00	0.00	3A7
ATOM	2990	CA	PHE	414	-0.981 -		19.200	1.00	0.00	3A7
ATOM	2991	СВ	PHE	414	-0.298 -		20.125	1.00	0.00	3A7
ATOM	2992	CG	PHE	414		-16.580	21.179	1.00	0.00	3A7
ATOM	2993	CD1	PHE	414	1.763 -	-17.214	20.878	1.00	0.00	3A7
ATOM	2994	CD2		414	0.126 -		22.505	1.00	0.00	3A7
ATOM	2995	CEl		414		-17.815	21.887	1.00	0.00	3A7
MOTA	2996		PHE	414		-17.148	23.513	1.00	0.00	3A7
ATOM	2997	CZ	PHE	414		-17.802	23.199	1.00	0.00 0.00	3A7 3A7
ATOM	2998	C	PHE	414	-2.045		19.981 20.697	1.00	0.00	3A7
ATOM	2999	0	PHE	414 415	-2.819 · -2.093 ·		19.847	1.00	0.00	3A7
ATOM ATOM	3000 3001	N CA	LEU	415	-3.087		20.488	1.00	0.00	3A7
ATOM	3002	CB	LEU	415	-4.201		19.504	1.00	0.00	3A7
ATOM	3003	CG	LEU	415	-5.081		18.954	1.00	0.00	3A7
ATOM	3004		LEU	415	-5.988		17.812	1.00	0.00	3A7
ATOM	3005		LEU	415	-5.911	_	20.058	1.00	0.00	3A7
ATOM	3006	С	LEU	415	-2.421	-21.064	20.998	1.00	0.00	3A7
ATOM	3007	0	LEU	415	-2.308		20.252	1.00	0.00	3A7
ATOM	3008	N	PRO	416	-2.010		22.271	1.00	0.00	3A7
ATOM	3009	CA	PRO	416	-1.339		22.847	1.00	0.00	3A7
MOTA	3010	CD	PRO	416	-1.874		23.122	1.00	0.00	3A7 3A7
ATOM	3011	CB	PRO	416	-1.071		24.299 24.207	1.00	0.00 0.00	3A7
ATOM	3012	CG	PRO	416 416	-0.878 -2.201		22.780	1.00	0.00	3A7
ATOM ATOM	3013 3014	C O	PRO PRO	416	-1.669		22.766	1.00	0.00	3A7
ATOM	3015	N	GLU	417		-23.381	22.682	1.00	0.00	3A7
ATOM	3016	CA	GLU	417		-24.458	22.678	1.00	0.00	3A7
ATOM	3017	СВ	GLU	417	•	-23.933	22.878	1.00	0.00	3A7
ATOM	3018	CG	GLU	417	-6.072	-23.126	24.179	1.00	0.00	3A7
ATOM	3019	CD	GLU	417		-22.672	24.323	1.00	0.00	3A7
ATOM	3020		GLU	417		-23.077	25.322	1.00	0.00	3A7
MOTA	3021	OE2		417		-21.911	23.436	1.00	0.00	3A7 3A7
MOTA	3022	C	GLU	417		-25.295	21.427 21.478	1.00	0.00 0.00	3A7
ATOM	3023	O N	GLU ARG	417 418		-26.446 -24.733	20.282	1.00	0.00	3A7
MOTA MOTA	3024 3025	CA	ARG	418		-25.279	18.944	1.00	0.00	. 3A7
ATOM	3026	СВ	ARG	418		-24.206	17.890	1.00	0.00	3A7
ATOM	3027	CG	ARG	418		-24.508	16.422	1.00	0.00	3A7
ATOM	3028	CD	ARG	418	-5.605	-24.343	16.069	1.00	0.00	3A7
ATOM	3029	NĘ	ARG	418	-6.397	-25.466	16.668	1.00	0.00	. 3A7
MOTA	3030	CZ	ARG	418		-25.471	16.670	1.00	0.00	3A7
MOTA	3031		ARG	418		-26.503	17.264	1.00	0.00	3A7
MOTA	3032		ARG	418		-24.456	16.087	1.00	0.00	3A7
ATOM	3033	C	ARG	418		-26.538 -26.489	18.706	1.00	0.00	3A7 3A7
ATOM	3034	0	ARG	418		-26.489	18.187 19.103	1.00	0.00	3A7
ATOM	3035 3036	N CA	PHE PHE	419 419		-29.076	18.984	1.00	0.00	3A7
ATOM ATOM	3037	CB	PHE	419		-29.565	17.516	1.00	0.00	3A7
ATOM	3038	CG	PHE	419		-29.517	16.915	1.00	0.00	3A7
ATOM	3039		PHE	419		-28.723	15.799	1.00	0.00	3A7
ATOM	3040		PHE	419	-5.806	-30.278	17.466	1.00	0.00	3A7
MOTA	3041	CE1	PHE	419	-6.325	-28.691	15.246	1.00	0.00	3A7
MOTA	3042		PHE	419		-30.245	16.919	1.00	0.00	3A7
ATOM	3043	CZ	PHE	419		-29.452	15.806		0.00	3A7
ATOM	3044	C	PHE	419		-29.334	19.681	1.00	0.00	3A7
ATOM	3045	0	PHE	419		-28.961	19.199		0.00	3A7
ATOM	3046	N	SER			-30.000	20.861		0.00	3A7 3A7
ATOM	3047	CA	SER			-30.259 -30.137	21.764		0.00	3A7
ATOM	3048	CB OG	SER SER			-30.137	24.172		0.00	3A7
ATOM ATOM	3049 3050	C	SER			-31.644	21.508			3A7
ATOM	3051	Ö	SER			-32.527	21.013			3A7
ATOM	3052	N	LYS			-31.842	21.877			3A7

MOTA	3053	CA	LYS	421	1.404 -	33.112	21.813	1.00	0.00	3A7
ATOM	3054	СВ	LYS	421	2.506 -		20.717	1.00	0.00	3A7
									0.00	3A7
ATOM	3055	CG	LYS	421	3.804 -		20.921			
ATOM	3056	CD	LYS	421	3.679 -	30.845	20.996	1.00	0.00	3A7
ATOM	3057	CE	LYS	421	3.332 -	30.147	19.673	1.00	0.00	3A7
ATOM	3058	NZ	LYS	421	1.927 -		19.273	1.00	0.00	3A7
						-				
MOTA	3059	С	LYS	421	2.007 -		23.167	1.00	0.00	3A7
ATOM	3060	0	LYS	421	2.165 -	32.424	23.962	1.00	0.00	3A7
ATOM	3061	N	LYS	422	2.373 ~	34.620	23.448	1.00	0.00	3A7
								1.00	0.00	3A7
MOTA	3062	CA	LYS	422	3.032 -		24.675			
MOTA	3063	CB	LY\$	422	2.048 -	35.203	25.856	1.00	0.00	3A7
MOTA	3064	CG	LYS	422	2.715 -	35.433	27.225	1.00	0.00	3A7
ATOM	3065	CD	LYS	422	3.520 -	34.222	27.727	1.00	0.00	3A7
	3066				4.151 -		29.109	1.00	0.00	3A7
ATOM		CE	LYS	422						
MOTA	3067	NZ	LYS	422	5.140 -	35.537	29.071	1.00	0.00	3A7
ATOM	3068	С	LYS	422	3.767 -	36.262	24.379	1.00	0.00	3A7
ATOM	3069	0	LYS	422	4.874 -	36.483	24.867	1.00	0.00	3A7
							23.555	1.00	0.00	3A7
ATOM	3070	N	ASN	423	3.138 -					
MOTA	3071	CA	ASN	423	3.658 -	-38.427	23.165	1.00	0.00	3A7
ATOM	3072	CB	ASN	423	2.646 -	-39.581	23.442	1.00	0.00	3A7
ATOM	3073	CG	ASN	423	1.264 -		22.812	1.00	0.00	3A7
ATOM	3074		ASN	423	0.498 -		23.277	1.00	0.00	3A7
ATOM	3075	ND2	ASN	423	0.950 -	-40.110	21.734	1.00	0.00	3A7
ATOM	3076	С	ASN	423	4.031 -	-38.367	21.703	1.00	0.00	3A7
					3.916 -		21.061	1.00	0.00	3A7
ATOM	3077	0	ASN	423						
MOTA	3078	N	LYS	424	4.481 -	-39.522	21.148	1.00	0.00	3A7
ATOM	3079	CA	LYS	424	4.861 -	-39.684	19.760	1.00	0.00	3A7
ATOM	3080	СВ	LYS	424	5.998 -	-40.724	19.591	1.00	0.00	3A7
						-40.859			0.00	3A7
ATOM	3081	CG	LYS	424			18.153	1.00		
MOTA	3082	CD	LYS	424	7.676 -	-41.874	18.013	1.00	0.00	3A7
ATOM	3083	CE	LYS	424	8.960 -	-41.460	18.744	1.00	0.00	3A7
ATOM	3084	NZ	LYS	424	10.027 -	-42.465	18.534	1.00	0.00	3A7
						-40.125	18.981	1.00	0.00	3A7
ATOM	3085	С	LYS	424						
ATOM	3086	0	LYS	424		-41.116	19.335	1.00	0.00	3A7
ATOM	3087	N	ASP	425	3.321 -	-39.353	17.910	1.00	0.00	3A7
MOTA	3088	CA	ASP	425	2.171 -	-39.492	17.032	1,00	0.00	3A7
ATOM	3089	СВ	ASP	425		-40.959	16.658	1.00	0.00	3A7
MOTA	3090	CG	ASP	425		-41.005	15.496	1.00	0.00	3A7
ATOM	3091	OD1	ASP	425	-0.322 -	-41.550	15.698	1.00	0.00	3A7
ATOM	3092	002	ASP	425	1.142 -	-40.497	14.397	1.00	0.00	3A7
				425		-38.771	17.679	1.00	0.00	3A7
ATOM	3093	C	ASP							
MOTA	3094	0	ASP	425	0.241	-39.355	18.444	1.00	0.00	3A7
ATOM	3095	N	ASN	426	0.881 -	-37.457	17.372	1.00	0.00	3A7
ATOM	3096	CA	ASN	426	-0.110 -	-36.573	17.945	1.00	0.00	3A7
ATOM	3097	СВ	ASN	426		-35.250	18.487	1.00	0.00	3A7
ATOM	3098	CG	ASN	426		-34.458	17.438	1.00	0.00	3A7
ATOM	3099	OD1	ASN	426	2.282	-34.963	16.848	1.00	0.00	3 A 7
ATOM	3100	ND2	ASN	426	0.912	-33.168	17.234	1.00	0.00	3A7
ATOM	3101	С	ASN	426	-1.189		16.915	1.00	0.00	3A7
					•					3A7
ATOM	3102	0	ASN	426	-1.547		16.157	1.00	0.00	
ATOM	3103	N	ILE	427	-1.746		16.880	1.00	0.00	3A7
ATOM	3104	CA	ILE	427	-2.849	-34.709	16.022	1.00	0.00	3A7
ATOM	3105	СВ	ILE	427	-3.731	-33 632	16.647	1.00	0.00	3A7
									0.00	3A7
ATOM	3106		ILE	427	-4.975		15.762	1.00		
ATOM	3107	CG1	ILE	427	-4.130	-34.009	18.097	1.00	0.00	3A7
ATOM	3108	CD	ILE	427	-4.944	-35.302	18.218	1.00	0.00	3A7
ATOM	3109	С	ILE	427	-2.306	-34.224	14.699	1.00	0.00	3A7
	3110				-2.782		13.641	1.00	0.00	3A7
ATOM		0	ILE	427						
ATOM	3111	N	ASP	428	-1.289		14.741	1.00	0.00	3A7
ATOM	3112	CA	ASP	428	-0.691	-32.752	13.555	1.00	0.00	3A7
ATOM	3113	СВ	ASP	428	-1.067		13.360	1.00	0.00	3A7
				428	-2.578		13.173	1.00	0.00	3A7
ATOM	3114	CG	ASP							
ATOM	3115		ASP	428	-3.101		12.169	1.00	0.00	3A7
MOTA	3116	OD2	ASP	428	-3.224	-30.473	14.030	1.00	0.00	3 A 7
ATOM	3117	С	ASP	428		-32.877	13.650	1.00	0.00	3A7
						-31.935		1.00	0.00	3A7
MOTA	3118	0	ASP	428			14.093			
ATOM	3119	N	PRO	429		-34.003	13.251	1.00	0.00	3A7
ATOM	3120	CA	PRO	429	2.856	-34.177	13.157	1.00	0.00	3A7
ATOM	3121	CD	PRO	429		-35.245	12.998	1.00	0.00	3A7
						-35.701	13.258	1.00	0.00	3A7
ATOM	3122	CB	PRO	429						
MOTA	3123	CG	PRO	429		-36.266	12.604	1.00	0.00	3A7
MOTA	3124	С	PRO	429	3.490	-33.658	11.858	1.00	0.00	3 A 7

ATOM	3125	0	PRO	429	2.892	-33.616	10.780	1.00	0.00	3A7
ATOM	3126	N	TYR	430		-33.325	11.967	1.00	0.00	3A7
ATOM	3127	CA	TYR	430	5.745	-33.153	10.884	1.00	0.00	3A7
ATOM	3128	СВ	TYR	430	5.621	-34.248	9.770	1.00	0.00	3A7
ATOM	3129	CG	TYR	430	6.889	-34.285	8.969	1.00	0.00	3A7
ATOM	3130	CD1	TYR	430	8.048	-34.836	9.516	1.00	0.00	3A7
ATOM	3131	CD2	TYR	430	6.967	-33.566	7.779	1.00	0.00	3A7
ATOM	3132	CEl	TYR	430	9.284	-34.596	8.926	1.00	0.00	3A7
ATOM	3133	CE2	TYR	430	8.205	-33.267	7.232	1.00	0.00	3A7
MOTA	3134	CZ	TYR	430	9.366	-33.774	7.806	1.00	0.00	3A7
ATOM	3135	OH	TYR	430	10.620		7.266	1.00	0.00	3A7
ATOM	3136	С	TYR	430		-31.761	10.274	1.00	0.00	3A7
ATOM	3137	0	TYR	430	6.683	-31.428	9.529	1.00	0.00	3A7
MOTA	3138	N	ILE	431		-30.877	10.599	1.00	0.00	3A7
ATOM	3139	CA	ILE	431		-29.502	10.146	1.00	0.00	3A7
ATOM	3140	СВ	ILE	431		-28.893	9.784	1.00	0.00	3A7
ATOM	3141		ILE	431		-29.661	8.570	1.00	0.00	3A7
ATOM	3142		ILE	431		-28.800	10.949	1.00	0.00	3A7
ATOM	3143	CD	ILE	431		-30.124	11.513	1.00	0.00	3A7
ATOM	3144	С	ILE	431		-28.630	11.193	1.00	0.00	3A7
ATOM	3145	0	ILE	431		-27.509	10.893	1.00	0.00	3A7
ATOM	3146	N	TYR	432		-29.122	12.460	1.00	0.00	3A7
ATOM	3147	CA	TYR	432		-28.443	13.571	1.00	0.00	3A7
ATOM	3148	CB	TYR	432		-28.969	14.973	1.00	0.00	3A7
ATOM	3149	CG	TYR	432		-28.367	15.505	1.00	0.00	3A7
ATOM	3150		TYR	432		-29.190	15.886	1.00	0.00	3A7
ATOM	3151		TYR	432		-27.004 -28.665	15.799	1.00	0.00	3A7 3A7
ATOM	3152		TYR	432		-26.477	16.575 16.484	1.00 1.00	0.00 0.00	3A7
ATOM	3153 3154	CZ	TYR TYR	432 432		-27.307	16.878	1.00	0.00	3A7
ATOM ATOM	3155	OH	TYR	432		-26.773	17.586	1.00	0.00	3A7
ATOM	3156	C	TYR	432		-28.741	13.531	1.00	0.00	3A7
ATOM	3157	Ö	TYR	432		-29.675	14.169	1.00	0.00	3A7
ATOM	3158	N	THR	433		-27.919	12.778	1.00	0.00	3A7
ATOM	3159	CA	THR	433		-28.119	12.506	1.00	0.00	3A7
MOTA	3160	СВ	THR	433		-28.167	10.995	1.00	0.00	3A7
ATOM	3161		THR	433		-26.980	10.336	1.00	0.00	3A7
ATOM	3162		THR	433		-29.368	10.401	1.00	0.00	3A7
ATOM	3163	С	THR	433		-27.070	13.107	1.00	0.00	3A7
ATOM	3164	0	THR	433	11.720	-26.744	12.459	1.00	0.00	3A7
MOTA	3165	N	PRO	434	10.544	-26.494	14.305	1.00	0.00	3A7
ATOM	3166	CA	PRO	434	11.476	-25.526	14.854	1.00	0.00	3A7
MOTA	3167	CĐ	PRO	434	9.603	-26.944	15.329	1.00	0.00	3A7
ATOM	3168	СB	PRO	434		-25.003	16.098	1.00	0.00	3A7
ATOM	3169	CG	PRO	434	9.981	-26.220	16.622	1.00	0.00	3A7
ATOM	3170	С	PRO	434		-26.180	15.226	1.00	0.00	3A7
ATOM	3171	0	PRO	434		-25.477	15.300	1.00	0.00	3A7
MOTA	3172	N	PHE	435		-27.518	15.456	1.00	0.00	3A7
MOTA	3173	CA	PHE	435	•	-28.253	15.844	1.00	0.00	3A7
MOTA	3174	CB	PHE	435		-29.173	17.045	1.00	0.00	3A7
ATOM	3175	CG	PHE	435		-28.509	18.358	1.00	0.00	3A7 3A7
ATOM	3176	CD1		435		-27.557	18.520 19.269	1.00	0.00	3A7 3A7
ATOM	3177 3178		PHE	435		-28.261 -26.403	19.460	1.00	0.00	3A7
ATOM ATOM	3178		PHE	435 435		-27.600	20.460	1.00	0.00	3A7
ATOM	3180	CZ	PHE	435		-26.726	20.695	1.00	0.00	3A7
ATOM	3181	C	PHE	435		-29.099	14.689	1.00	0.00	3A7
ATOM	3182	ŏ	PHE	435		-29.980	14.855	1.00	0.00	3A7
ATOM	3183	N	GLY	436		-28.834	13.469	1.00	0.00	3A7
ATOM	3184	CA	GLY	436		-29.495	12.269	1.00	0.00	3A7
ATOM	3185	Ċ	GLY	436		-30.777	12.129	1.00	0.00	3A7
ATOM	3186	ŏ	GLY	436		-31.061	12.870	1.00	0.00	3A7
ATOM	3187	N	SER			-31.599	11.152	1.00	0.00	3A7
ATOM	3188	CA	SER			-32.872	10.944	1.00	0.00	3A7
ATOM	3189	СВ	SER			-32.829	9.974	1.00	0.00	3A7
ATOM	3190	OG	SER			-32.079	10.518	1.00	0.00	3A7
ATOM	3191	С	SER		14.585	-33.730	10.351	1.00	0.00	3A7
MOTA	3192	0	SER		15.352	-33.291	9.494	1.00	0.00	3A7
ATOM	3193	N	GLY	438	14.623	-35.006	10.788			3A7
MOTA	3194	CA	GLY			-36.010	10.184			3A7
MOTA	3195	С	GLY			-36.414	11.067			3A7
MOTA	3196	0	GLY	438	16.526	-36.346	12.293	1.00	0.00	3A7

MOTA	3197	N	PRO	439	17.704 -3	6.873	10.443		0.00	3A7
ATOM	3198	CA	PRO	439	18.897 -3		11.180		0.00	3A7
MOTA	3199	CD	PRO	439	17.653 -3		9.152		0.00	3A7 3A7
ATOM	3200	CB	PRO	439 439	19.741 -3 18.702 -3		10.170 9.220		0.00 0.00	3A7
MOTA MOTA	3201 3202	CG C	PRO PRO	439	19.700 -3		11.729		0.00	3A7
ATOM	3203	ŏ	PRO	439	20.523 -3		12.614	1.00	0.00	3A7
ATOM	3204	N	ARG	440	19.490 -3		11.217	1.00	0.00	3A7
ATOM	3205	CA	ARG	440	20.212 -3	33.720	11.642	1.00	0.00	3A7
MOTA	3206	CB	ARG	440	20.704 -3		10.433	1.00	0.00	3A7
ATOM	3207	CG	ARG	440	21.775 -		9.617	1.00	0.00	3A7
ATOM	3208	CD	ARG	440	21.846 -3		8.148 7.458	1.00	0.00	3A7 3A7
ATOM ATOM	3209 3210	NE CZ	ARG ARG	440 440	20.618 -: 20.391 -:		6.123	1.00	0.00	3A7
ATOM	3211	NH1		440	19.299 -		5.537	1.00	0.00	3A7
ATOM	3212	NH2		440	21.244 -		5.371	1.00	0.00	3A7
ATOM	3213	С	ARG	440	19.307 -	32.855	12.480	1.00	0.00	3A7
MOTA	3214	0	ARG	440	19.471 -		12.565	1.00	0.00	3A7
MOTA	3215	N	ASN	441	18.322 -		13.163	1.00	0.00	3A7
ATOM	3216	CA	ASN	441	17.420 -		14.066	1.00	0.00	3A7 3A7
ATOM	3217 3218	CB CG	ASN ASN	441 441	16.263 - 16.713 -		14.515 15.324	1.00	0.00	3A7
ATOM ATOM	3219		ASN	441	17.527 -		14.869	1.00	0.00	3A7
ATOM	3220		ASN	441	16.154 -		16.567	1.00	0.00	3A7
ATOM	3221	С	ASN	441	18.197 -		15.260	1.00	0.00	3A7
ATOM	3222	0	ASN	441	19.263 -		15.550	1.00	0.00	3A7
ATOM	3223	N	CYS	442	17.690 -		15.990	1.00	0.00	3A7
ATOM	3224	CA	CYS	442	18.409 - 17.629 -		17.097 17.676	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	3225 3226	CB SG	CYS CYS	442 442	18.592 -		18.905	1.00	0.00	3A7
ATOM	3227	c	CYS	442	18.683 -		18.181	1.00	0.00	3A7
ATOM	3228	ō	CYS	442	17.779 -		18.699	1.00	0.00	3A7
ATOM	3229	N	ILE	443	19.971 -	31.894	18.535	1.00	0.00	3A7
MOTA	3230	CA	ILE	443	20.405 -		19.531	1.00	0.00	3A7
ATOM	3231	CB	ILE	443	21.872 -		19.324	1.00	0.00	3A7 3A7
MOTA	3232		ILE	443 443	22.414 ~ 22.046 ~		20.472 17.955	1.00	0.00 0.00	3A7
ATOM ATOM	3233 3234	CD	ILE	443	21.378 -		17.849	1.00	0.00	3A7
ATOM	3235	c	ILE	443	20.167 -		20.902	1.00	0.00	3A7
ATOM	3236	Ō	ILE	443	20.008 -	32.929	21.894	1.00	0.00	3A7
ATOM	3237	N	GLY	444	20.106 -		20.975	1.00	0.00	3A7
MOTA	3238	CA	GLY	444	19.894 -		22.204	1.00	0.00	3A7 3A7
ATOM	3239	C	GLY	444 444	18.471 - 18.222 -		22.535 23.479	1.00	0.00	3A7
ATOM ATOM	3240 3241	O N	GLY MET	445	17.493 -		21.788	1.00	0.00	3A7
ATOM	3242	CA	MET	445	16.056 -		21.939	1.00	0.00	3A7
ATOM	3243	СВ	MET	445	15.279 -	31.201	21.002	1.00	0.00	3A7
ATOM	3244	CG	MET	445	13.742 -		21.137	1.00	0.00	3A7
MOTA	3245	SD	MET	445	12.898 -		19.780	1.00	0.00	3A7 3A7
ATOM	3246 3247	CE	MET MET	445 445	13.584 - 15.558 -		20.107	1.00	0.00	3A7
ATOM ATOM	3247	С 0	MET	445	14.887 -		23.919	1.00	0.00	3A7
ATOM	3249	N	ARG	446	15.928 -		23.976	1.00	0.00	3A7
ATOM	3250	CA	ARG	446	15.476 -	-31.910	25.309	1.00	0.00	3A7
MOTA	3251	СВ	ARG	446	15.826 -		25.684	1.00	0.00	3A7
ATOM	3252	CG	ARG	446	15.490 -		24.538	1.00	0.00	3A7 3A7
MOTA	3253	CD	ARG	446	15.588 - 14.428 -		24.911 25.799	1.00	0.00	3A7
ATOM ATOM	3254 3255	NE CZ	ARG ARG	446 446	14.005		25.986	1.00	0.00	3A7
ATOM	3256		ARG	446	12.921		26.780	1.00	0.00	3A7
ATOM	3257		ARG	446	14.658		25.394	1.00	0.00	3A7
ATOM	3258	C	ARG	446	16.001	-30.952	26.348	1.00	0.00	3A7
ATOM	3259	0	ARG		15.276		27.248	1.00	0.00	3A7
ATOM	3260	N	PHE		17.267		26.201	1.00	0.00	3A7 3A7
ATOM	3261 3262	CA CB	PHE		17.865 19.408		27.113 27.061	1.00		3A7
ATOM ATOM	3263	CG	PHE		19.952		26.613		0.00	3A7
ATOM	3264		PHE		20.810		25.520			3A7
MOTA	3265		PHE		19.433	-32.037	27.086	1.00		3A7
ATOM	3266		PHE		20.971		24.778			3A7
ATOM	3267		PHE		19.526		26.291			3A7 3A7
ATOM	3268	CZ	PHE	447	20.229	-33.109	25.096	1.00	0.00	JA/

MOTA	3269	С	PHE	447	17.285 -28.185	26.918	1.00	0.00	3A7
ATOM	3270	0	PHE	447	17.071 -27.458	27.881	1.00	0.00	3A7
ATOM	3271	N	ALA	448	16.949 -27.798	25.656	1.00	0.00	3A7
ATOM	3272	CA	ALA	448	16.406 -26.493	25.374	1.00	0.00	3A7
ATOM	3273	CB	ALA	448	16.379 -26.216	23.882	1.00	0.00	3A7
MOTA	3274	С	ALA	448	15.020 -26.344	25.914	1.00	0.00	3A7
MOTA	3275	0	ALA	448	14.679 -25.313	26.493	1.00	0.00	3A7
MOTA	3276	N	LEU	449	14.197 -27.406	25.800	1.00	0.00	3A7
MOTA	3277	CA	LEU	449	12.842 -27.402	26.309	1.00	0.00	3A7
ATOM	3278	CB	LEU	449	12.029 -28.605	25.813	1.00	0.00	3A7
ATOM	3279	CG	LEU	449	11.639 -28.523 11.120 -29.879	24.324	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	3280 3281	CD1		449 449	10.621 -27.401	23.807 24.038	1.00	0.00	3A7 3A7
MOTA	3282	CDZ	LEU	449	12.800 -27.422	27.811	1.00	0.00	3A7
ATOM	3283	ŏ	LEU	449	11.936 -26.797	28.417	1.00	0.00	3A7
ATOM	3284	N	VAL	450	13.770 -28.111	28.454	1.00	0.00	3A7
MOTA	3285	CA	VAL	450	13.883 -28.171	29.893	1.00	0.00	3A7
ATOM	3286	СВ	VAL	450	14.890 -29.213	30.345	1.00	0.00	3A7
ATOM	3287	CG1	VAL	450	15.177 -29.141	31.862	1.00	0.00	3A7
ATOM	3288	CG2	VAL	450	14.262 -30.592	30.049	1.00	0.00	3A7
ATOM	3289	С	VAL	450	14.256 -26.828	30.431	1.00	0.00	3A7
ATOM	3290	0	VAL	450	13.633 -26.345	31.364	1.00	0.00	3A7
MOTA	3291	N	ASN	451	15.263 -26.162	29.833	1.00	0.00	3A7
ATOM	3292	CA	ASN	451	15.735 -24.855	30.232	1.00	0.00	3A7
ATOM	3293	CB	ASN	451	16.873 -24.401	29.295	1.00	0.00	3A7 3A7
MOTA	3294	CG	ASN	451	18.141 -25.243	29.476 30.369	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	3295 3296		ASN ASN	451 451	18.233 -26.089 19.145 -24.981	28.583	1.00	0.00	3A7
ATOM	3297	C	ASN	451	14.659 -23.792	30.150	1.00	0.00	3A7
ATOM	3298	ŏ	ASN	451	14.440 -23.023	31.081	1.00	0.00	3A7
ATOM	3299	N	MET	452	13.918 -23.759	29.019	1.00	0.00	3A7
MOTA	3300	CA	MET	452	12.853 -22.808	28.800	1.00	0.00	3A7
ATOM	3301	CB	MET	452	12.311 -22.880	27.353	1.00	0.00	3A7
MOTA	3302	CG	MET	452	13.202 -22.090	26.370	1.00	0.00	3A7
MOTA	3303	SD	MET	452	13.800 -22.975	24.894	1.00	0.00	3A7
ATOM	3304	CE	MET	452	12.280 -23.810	24.359	1.00	0.00	3A7
ATOM	3305	C	MET	452	11.733 -22.982	29.778	1.00	0.00	3A7 3A7
ATOM ATOM	3306 3307	O N	MET Lys	452 453	11.255 -22.013 11.310 -24.236	30.355 30.042	1.00	0.00	3A7
ATOM	3308	CA	LYS	453	10.240 -24.536	30.965	1.00	0.00	3A7
ATOM	3309	СВ	LYS	453	9.864 -26.021	30.868	1.00	0.00	3A7
ATOM	3310	CG	LYS	453	8.486 -26.409	31.399	1.00	0.00	3A7
ATOM	3311	CD	LYS	453	8.218 -27.911	31.258	1.00	0.00	3A7
ATOM	3312	CE	LYS	453	8.280 -28.457	29.817	1.00	0.00	3A7
ATOM	3313	NZ	LYS	453	9.661 -28.675	29.322	1.00	0.00	3A7
ATOM	3314	С	LYS LYS	453 453	10.616 -24.214 9.869 -23.577	32.386 33.112	1.00	0.00	3A7 3A7
ATOM ATOM	3315 3316	O N	LEU	454	11.836 -24.594	32.812	1.00	0.00	3A7
ATOM	3317	CA)	LEU	454	12.304 -24.349		1.00	0.00	3A7
ATOM	3318	СВ	LEU	454	13.614 -25.110		1.00	0.00	3A7
MOTA	3319	CG	LEU	454	13.420 -26.655	34.462	1.00	0.00	3A7
MOTA	3320		LEU	454	14.712 -27.380				3A7
ATOM	3321		LEU	454	,12.265 -27.101		1.00	0.00	3A7
MOTA	3322	C	LEU	454	12.488 -22.881		1.00	0.00	3A7
MOTA MOTA	3323 3324	0	LEU	454 455	12.033 -22.383 13.101 -22.129		1.00	0.00 0.00	3A7 3A7
ATOM	3325	N CA	ALA ALA	455	13.303 -20.699		1.00	0.00	3A7
ATOM	3326	CB	ALA	455	14.157 -20.149		1.00	0.00	3A7
ATOM	3327	c	ALA	455	12.006 -19.916		1.00		3A7
ATOM	3328	0	ALA	455	11.803 -19.112	34.569	1.00	0.00	3A7
MOTA	3329	N	LEU	456	11.065 -20.169	32.730	1.00		3A7
ATOM	3330	CA	LEU	456	9.795 -19.468		1.00	0.00	3A7
ATOM	3331	CB	LEU	456	9.033 -19.835		1.00		3A7
ATOM	3332	CG CD1	LEU	456 456	9.514 -19.139 10.961 -18.619		1.00		3A7 3A7
ATOM ATOM	3333 3334		LEU	456 456	9.277 -20.054		1.00		3A7 3A7
ATOM	3335	CD2	LEU	456	8.902 -19.770		1.00		3A7
ATOM	3336	ŏ	LEU	456	8.226 -18.888		1.00		3A7
ATOM	3337	N	VAL	457	8.933 -21.025		1.00		3A7
ATOM	3338	CA	VAL	457	8.191 -21.445		1.00	0.00	3A7
MOTA	3339	СВ	VAL	457	8.444 -22.911		1.00		3A7
MOTA	3340	CG1	VAL	457	8.005 -23.325	37.263	1.00	0.00	3A7

MOTA	3341	CG2	VAL	457	7.670	-23.765	34.841	1.00	0.00	3A7
ATOM	3342	С	VAL	457		-20.633	36.694	1.00	0.00	3A7
ATOM	3343	ō	VAL	457		-20.161	37.444	1.00	0.00	3A7
ATOM	3344			458					0.00	
		N	ARG			-20.443	36.892	1.00		3A7
ATOM	3345	CA	ARG	458		-19.722	38.015	1.00	0.00	3A7
MOTA	3346	CB	ARG	458	11.926	-19.996	38.164	1.00	0.00	3A7
ATOM	3347	CG	ARG	458	12.246	-21.369	38.758	1.00	0.00	3A7
ATOM	3348	CD	ARG	458	13.750	-21.581	38.977	1.00	0.00	3A7
MOTA	3349	NE	ARG	458		-21.751	37.641	1.00	0.00	3A7
ATOM	3350	CZ	ARG	458		-22.941	37.197	1.00	0.00	3A7
ATOM	3351	NH1		458		-22.979	35.995	1.00	0.00	3A7
MOTA	3352	NH2		458		-24.080	37.937	1.00	0.00	3A7
ATOM	3353	С	ARG	458	10.219	-18.233	37.894	1.00	0.00	3A7
MOTA	3354	0	ARG	458	9.873	-17.578	38.869	1.00	0.00	3A7
ATOM	3355	N	VAL	459	10.398	-17.640	36.691	1.00	0.00	3A7
ATOM	3356	CA	VAL	459	10.219	-16.217	36.448	1.00	0.00	3A7
ATOM	3357	СВ	VAL	459		-15.894	35.017	1.00	0.00	3A7
MOTA	3358	CG1		459		-14.508	34.526	1.00	0.00	3A7
MOTA	3359		VAL	459		-16.014	34.950	1.00	0.00	3A7
ATOM	3360	С	VAL	459	8.793	-15.789	36.752	1.00	0.00	3A7
ATOM	3361	0	VAL	459	8.553	-14.855	37.511	1.00	0.00	3A7
ATOM	3362	N	LEU	460	7.804	-16.538	36.226	1.00	0.00	3A7
ATOM	3363	CA	LEU	460		-16.237	36.374	1.00	0.00	3A7
ATOM	3364	СВ	LEU	460		-17.011	35.340	1.00	0.00	3A7
ATOM	3365	CG	LEU	460		-16.588	33.893	1.00	0.00	3A7
ATOM	3366	CD1		460		-17.596	32.898	1.00	0.00	3A7
MOTA	3367	CD2	LEU	460	5.418	-15.150	33.610	1.00	0.00	3A7
ATOM	3368	С	LEU	460	5.857	-16.582	37.736	1.00	0.00	3A7
ATOM	3369	0	LEU	460	4.817	-16.068	38.141	1.00	0.00	3A7
ATOM	3370	N	GLN	461		-17.449	38.498	1.00	0.00	3A7
ATOM	3371	CA	GLN	461		-17.756	39.877	1.00	0.00	3A7
	3372	СВ								
MOTA			GLN	461		-19.025	40.414	1.00	0.00	3A7
ATOM	3373	CG	GLN	461		-19.729	41.554	1.00	0.00	3A7
ATOM	3374	CD	GLN	461	6.924	-21.033	41.909	1.00	0.00	3A7
ATOM	3375	OE1	GLN	461	7.856	-21.463	41.220	1.00	0.00	3A7
ATOM	3376	NE2	GLN	461	6.464	-21.670	43.029	1.00	0.00	3A7
ATOM	3377	С	GLN	461	6.618	-16.632	40.808	1.00	0.00	3A7
ATOM	3378	0	GLN	461		-16.385	41.809	1.00	0.00	3A7
ATOM	3379	N	ASN	462		-15.950	40.487	1.00	0.00	3A7
ATOM	3380	CA	ASN	462						
						-15.014	41.373	1.00	0.00	3A7
ATOM	3381	СВ	ASN	462		-15.166	41.353	1.00	0.00	3A7
ATOM	3382	CG	ASN	462		-16.436	42.117	1.00	0.00	3A7
ATOM	3383	OD1	ASN	462	10.091	-17.563	41.666	1.00	0.00	3A7
ATOM	3384	ND2	ASN	462	10.944	-16.227	43.317	1.00	0.00	3A7
ATOM	3385	С	ASN	462	8.026	-13.582	41.041	1.00	0.00	3A7
ATOM	3386	0	ASN	462		-12.710	41.888	1.00	0.00	3A7
ATOM	3387	N	PHE	463		-13.284	39.807	1.00	0.00	3A7
ATOM	3388	CA	PHE	463		-11.906				3A7
	3389						39.372	1.00	0.00	
ATOM		CB	PHE	463	•	-11.416	38.535	1.00	0.00	3A7
ATOM	3390	CG	PHE	463		-11.494	39.308	1.00	0.00	3A7
MOTA	3391		PHE	463	10.834	-12.474	38.996	1.00	0.00	3A7
ATOM	3392	CD2	PHE	463	10.162	-10.594	40.340	1.00	0.00	3A7
ATOM	3393	CE1	PHE	463	12.021	-12.568	39.714	1.00	0.00	3A7
ATOM	3394	CE2	PHE	463		-10.684	41.057	1.00	0.00	3A7
ATOM	3395	CZ	PHE	463		-11.673	40.747	1.00	0.00	3A7
ATOM '	3396	c	PHE	463		-11.715	38.530	1.00	0.00	3A7
ATOM	3397									
		0	PHE	463		-12.637	37.862	1.00	0.00	3A7
ATOM	3398	N	SER	464		-10.452	38.530	1.00	0.00	3A7
MOTA	3399	CA	SER	464	4.607	-9.957	37.639	1.00	0.00	3A7
ATOM	3400	СВ	SER	464	3.437	-9.228	38.330	1.00	0.00	3A7
ATOM	3401	OG	SER	464	3.854	-8.156	39.167	1.00	0.00	3A7
ATOM	3402	С	SER	464	5.295	-9.043	36.654	1.00	0.00	3A7
ATOM	3403	ō	SER	464	5.987		37.035	1.00	0.00	3A7
ATOM	3404	N	PHE	465	5.122	-9.324	35.343		0.00	3A7
								1.00		
ATOM	3405	CA	PHE	465	5.823		34.275	1.00	0.00	3A7
ATOM	3406	СВ	PHE	465	6.320		33.195	1.00	0.00	3A7
MOTA	3407	CG	PHE	465		-10.312	33.835	1.00	0.00	3A7
MOTA	3408	CD1	PHE	465	7.317	-11.547	34.451	1.00	0.00	3A7
ATOM	3409	CD2	PHE	465	8.689	-9.634	33.959	1.00	0.00	3A7
ATOM	3410		PHE	465		-12.080	35.204	1.00	0.00	3A7
ATOM	3411		PHE	465		-10.176	34.692	1.00	0.00	3A7
ATOM	3412	CZ	PHE	465		-11.399	35.322	1.00	0.00	3A7
A L OFF	7-12				9.504	11.333	33.342	1.00	0.00	JA /

ATOM	3413	С	PHE	465	4.919	-7.687	33.592	1.00	0.00	3A7
ATOM	3414	0	PHE	465	3.724	-7.936	33.425	1.00	0.00	3A7
ATOM	3415	N	LYS	466	5.493	-6.560	33.115	1.00	0.00	3A7
ATOM	3416	CA	LYS	466	4.734	-5.582	32.382	1.00	0.00	3A7
ATOM	3417	СВ	LYS	466	4.290	-4.427	33.296	1.00	0.00	3A7
ATOM	3418	CG	LYS	466	3.397	-4.837	34.480	1.00	0.00	3A7
ATOM	3419	CD	LYS	466	2.972	-3.643	35.348	1.00	0.00	3A7
		CE	LYS	466	2.140	-4.046	36.574	1.00	0.00	3A7
ATOM	3420							1.00		3A7
ATOM	3421	NZ	LYS	466	2.919	-4.922	37.481		0.00	
ATOM	3422	С	LYS	466	5.602	-5.043	31.290	1.00	0.00	3A7
ATOM	3423	0	LYS	466	6.771	-4.756	31.526	1.00	0.00	3A7
MOTA	3424	N	PRO	467	5.061	-4.811	30.080	1.00	0.00	3A7
MOTA	3425	CA	PRO	467	5.708	-4.063	29.024	1.00	0.00	3A7
ATOM	3426	CD	PRO	467	3.897	-5.529	29.577	1.00	0.00	3A7
MOTA	3427	CB	PRO	467	4.867	-4.318	27.759	1.00	0.00	3A7
ATOM	3428	CG	PRO	467	4.104	-5.604	28.064	1.00	0.00	3A7
ATOM	3429	С	PRO	467	5.709	-2.585	29.358	1.00	0.00	3A7
ATOM	3430	0	PRO	467	4.657	-2.040	29.696	1.00	0.00	3A7
ATOM	3431	N	CYS	468	6.875	-1.912	29.284	1.00	0.00	3A7
ATOM	3432	CA	CYS	468	7.012	-0.524	29.684	1.00	0.00	3A7
ATOM	3433	СВ	CYS	468	8.466	-0.147	30.062	1.00	0.00	3A7
ATOM	3434	SG	CYS	468	9.057	-1.091	31.487	1.00	0.00	3A7
ATOM	3435	C	CYS	468	6.616	0.383	28.544	1.00	0.00	3A7
ATOM	3436	ŏ	CYS	468	6.411	1.583	28.713	1.00	0.00	3A7
ATOM	3437	N	LYS	469	6.540	-0.205	27.334	1.00	0.00	3A7
	3438			469	6.355	0.499	26.104	1.00	0.00	3A7
ATOM	-	CA	LYS							3A7
ATOM	3439	CB	LYS	469	7.640	0.501	25.281	1.00	0.00	
ATOM	3440	CG	LYS	469	8.757	1.350	25.918	1.00	0.00	3A7
ATOM	3441	CD	LYS	469	10.000	1.530	25.028	1.00	0.00	3A7
ATOM	3442	CE	LYS	469	9.788	2.435	23.807	1.00	0.00	3A7
ATOM	3443	NZ	LYS	469	9.393	3.802	24.218	1.00	0.00	3A7
MOTA	3444	С	LYS	469	5.347	-0.291	25.354	1.00	0.00	3A7
ATOM	3445	0	LYS	469	5.575	-1.459	25.050	1.00	0.00	3A7
ATOM	3446	N	GLU	470	4.138	0.226	25.134	1.00	0.00	3A7
MOTA	3447	CA	GLU	470	3.141	-0.604	24.504	1.00	0.00	3A7
MOTA	3448	СВ	GLU	470	1.701	-0.299	24.997	1.00	0.00	3A7
ATOM	3449	CG	GLU	470	1.488	-0.619	26.491	1.00	0.00	3A7
MOTA	3450	CD	GLU	470	1.553	-2.121	26.773	1.00	0.00	3A7
ATOM	3451	OE1	GLU	470	1.559	-2.928	25.806	1.00	0.00	3A7
ATOM	3452	OE2	GLU	470	1.584	-2.480	27.981	1.00	0.00	3A7
ATOM	3453	С	GLU	470	3.348	-0.317	23.071	1.00	0.00	3A7
MOTA	3454	0	GLU	470	4.315	-0.740	22.429	1.00	0.00	3A7
ATOM	3455	N	THR	471	2.368	0.501	22.575	1.00	0.00	3A7
ATOM	3456	CA	THR	471	2.160	1.284	21.360	1.00	0.00	3A7
ATOM	3457	СB	THR	471	2.447	2.764	21.659	1.00	0.00	3A7
ATOM	3458		THR	471	1.929	3.641	20.661	1.00	0.00	3A7
ATOM	3459		THR	471	3.946	3.049	21.904	1.00	0.00	3A7
ATOM	3460	C	THR	471	2.841	0.808	20.088	1.00	0.00	3A7
	3461	Ö	THR	471	3.308	1.608	19.278	1.00	0.00	3A7
ATOM	3462	N			2.875	-0.535	19.884	1.00	0.00	3A7
ATOM			GLN	472			18.731	1.00	0.00	3A7
ATOM	3463	CA	GLN	472	3.410	-1.235			0.00	3A7
ATOM	3464	CB	GLN	472	2.623	-0.915	17.428	1.00	0.00	
ATOM	3465	CG	GLN	472	2.830	-1.913	16.270	1.00		3A7
ATOM	3466	CD	GLN	472	2.412	-3.322	16.703	1.00	0.00	3A7
ATOM	3467		GLN	472	3.252	-4.222	16.818	1.00	0.00	3A7
ATOM	3468		GLN	472	1.077	-3.502	16.944	1.00	0.00	3A7
ATOM	3469	С	GLN	472	4.893	-0.974	18.547	1.00	0.00	3A7
ATOM	3470	0	GLN	472	5.362	-0.673	17.450	1.00	0.00	3A7
ATOM	3471	N	ILE	473	5.672	-1.090	19.658	1.00	0.00	3A7
MOTA	3472	CA	ILE	473	7.130	-0.993	19.613	1.00	0.00	3A7
MOTA	3473	CB	ILE	473	7.790	-0.303	20.808	1.00	0.00	3A7
ATOM	3474	CG2	ILE	473	9.304	-0.020	20.648	1.00	0.00	3A7
ATOM	3475		ILE	473	7.030	1.009	21.146	1.00	0.00	3A7
ATOM	3476	CD	ILE	473	7.180	2.124	20.104	1.00	0.00	3A7
ATOM	3477	C	ILE	473	7.840	-2.153	19.174	1.00	0.00	3A7
ATOM	3478	ō	ILE	473	8.886	-1.850	18.619	1.00	0.00	3A7
ATOM	3479	N	PRO	474	7.388	-3.403	19.312	1.00	0.00	3A7
ATOM	3480	CA	PRO		8.307	-4.483	19.289	1.00		3A7
ATOM	3481	CD	PRO		6.293	-3.751	20.216	1.00		3A7
ATOM	3482	СВ	PRO		7.554	-5.688	19.660	1.00		3A7
ATOM	3483	CG	PRO		6.580	-5.162	20.707	1.00		3A7
ATOM	3484	C	PRO		9.042	-4.735		1.00		3A7
V1013	2404	-	- 10	7.14	3.042	-4.733	10.013	2.00	5.00	JA

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ATOM	3485		PRO	474	8.461	-4.845	16.967		0.00	3A7
MOTA	3486		LEU	475	10.363	-4.780	18.250		0.00	3A7 3A7
ATOM	3487		LEU	475	11.281 12.494	-4.868 -3.929	17.212 17.438	1.00	0.00	3A7
ATOM ATOM	3488 3489	CB CG	LEU	475 475	12.127	-2.431	17.558	1.00	0.00	3A7
MOTA	3490	CD1		475	13.371	-1.592	17.906	1.00	0.00	3A7
ATOM	3491	CD2		475	11.432	-1.891	16.293	1.00	0.00	3A7
MOTA	3492	С	LEU	475	11.786	-6.229	17.109	1.00	0.00	3A7
MOTA	3493	0	LEU	475	12.315	-6.781	18.064	1.00	0.00	3A7 3A7
ATOM	3494 3495	N CA	LYS LYS	476 476	11.627 12.112	-6.792 -8.088	15.915 15.588	1.00	0.00	3A7
MOTA MOTA	3496	CB	LYS	476	11.115	-8.801	14.712	1.00	0.00	3A7
ATOM	3497	CG	LYS	476	9.772	-9.009	15.441	1.00	0.00	3A7
MOTA	3498	CD	LYS	476	8.674	-9.612	14.555	1.00	0.00	3A7
MOTA	3499	CE	LYS	476		-11.068	14.167	1.00	0.00	3A7 3A7
ATOM	3500 3501	NZ C	LYS LYS	476 476	13.325	-11.545 -7.870	13.235 14.776	1.00	0.00	3A7
ATOM ATOM	3501	ō	LYS	476	13.323	-7.042	13.874	1.00	0.00	3A7
ATOM	3503	Ň	LEU	477	14.395	-8.621	15.042	1.00	0.00	3A7
MOTA	3504	CA	LEU	477	15.554	-8.551	14.210	1.00	0.00	3A7
MOTA	3505	CB	LEU	477	16.856	-8.930	14.889	1.00	0.00	3A7
ATOM	3506	CG CD1	LEU LEU	477	18.083 19.159	-8.017 -8.239	14.617 15.698	1.00 1.00	0.00	3A7 3A7
ATOM ATOM	3507 3508		LEU	477 477	18.705	-8.182	13.223	1.00	0.00	3A7
ATOM	3509	C	LEU	477	15.422	-9.412	13.099	1.00	0.00	3A7
MOTA	3510	0	LEU	477	14.926	-10.517	13,208	1.00	0.00	3A7
MOTA	3511	N	ARG	478	15.810	-8.885	11.967	1.00	0.00	3A7
ATOM	3512	CA	ARG	478	15.460	-9.604	10.853 9.829	1.00 1.00	0.00	3A7 3A7
MOTA MOTA	3513 3514	CB CG	ARG ARG	478 478	14.781 13.512	-8.647 -7.955	10.358	1.00	0.00	3A7
ATOM	3515	CD	ARG	478	12.226	-8.561	9.784	1.00	0.00	3A7
ATOM	3516	NE	ARG	478	12.180	-10.004	10.198	1.00	0.00	3A7
MOTA	3517	CZ	ARG	478	11.186		10.977	1.00	0.00	3A7
ATOM	3518		ARG	478		-11.836	11.366	1.00	0.00	3A7 3A7
ATOM ATOM	3519 3520	NH2 C	ARG ARG	478 478	10.121	-9.764 -10.335	11.352 10.080	1.00	0.00	3A7
ATOM	3521	ŏ	ARG	478		-10.652	8.927	1.00	0.00	3A7
ATOM	3522	N	PHE	479		-10.610	10.632	1.00	0.00	3A7
MOTA	3523	CA	PHE	479		-10.706	9.806	1.00	0.00	3A7
ATOM	3524	CB	PHE	479		-10.235 -9.680	10.539 9.633	1.00	0.00	3A7 3A7
ATOM ATOM	3525 3526	CG	PHE	479 479	21.147 20.917	-8.497	8.929	1.00	0.00	3A7
ATOM	3527		PHE	479		-10.322	9.495	1.00	0.00	3A7
ATOM	3528		PHE	479	21.894	-7.970	8.093	1.00	0.00	3A7
MOTA	3529		PHE	479	23.356	-9.799	8.652	1.00	0.00	3A7
ATOM	3530	CZ	PHE	479	23.115	-8.622 -12.054	7.951 9.251	1.00	0.00 0.00	3A7 3A7
ATOM ATOM	3531 3532	c o	PHE	479 479		-12.120	8.413	1.00	0.00	3A7
ATOM	3533	N	GLY	480		-13.153	9.632	1.00	0.00	3A7
ATOM	3534	CA	GLY	480		-14.416	8.969	1.00	0.00	3A7
MOTA	3535	С	GLY	480		-15.080	9.499	1.00	0.00	3A7 3A7
ATOM	3536 3537	N N	GLY GLY	480 481		-14.455 -16.400	9.781 9.691	1.00	0.00	3A7
ATOM ATOM	3538	CA	GLY	481		-17.199	10.480	1.00	0.00	3A7
ATOM	3539	Č.	GLY	481		-17.404	11.756	1.00	0.00	3A7
ATOM	3540	0	GLY	481		-18.530	12.126	1.00	0.00	3A7
MOTA	3541	N	LEU	482		-16.297	12.465	1.00	0.00	3A7 3A7
ATOM	3542	CA	LEU	482		-16.393 -16.416	13.801 14.840	1.00	0.00	3A7
ATOM ATOM	3543 3544	CB CG	LEU	482 482		-17.132	16.175	1.00	0.00	3A7
ATOM	3545		LEU	482		-16.443	17.020	1.00	0.00	3A7
MOTA	3546		LEU	482		-18.634	15.963	1.00	0.00	3A7
ATOM	3547	С	LEU	482		-15.192	13.998		0.00	3A7
ATOM	3548	0	LEU	482		-14.069 -15.412				3A7 3A7
MOTA MOTA	3549 3550		LEU	483 483		-14.371				3A7
ATOM	3551	СВ	LEU	483		-14.799				3A7
ATOM	3552		LEU	483	14.356	-14.905	12.543			3A7
ATOM	3553		LEU	483		-15.253				3A7
ATOM	3554		LEU	483		-13.634				3A7 3A7
MOTA MOTA	3555 3556		LEU LEU	483 483		-14.055 -14.926				3A7
W 1 OL1	2220	9			20.,00					

ATOM	3557	N	LEU	484	16.246	-12.778	16.236	1.00	0.00	3A7
ATOM	3558	CA	LEU	484	16.374		17.588	1.00	0.00	3A7
ATOM	3559	СВ	LEU	484	17.753		17.812	1.00	0.00	3A7
							17.710	1.00	0.00	3A7
MOTA	3560	CG	LEU	484	18.984					
MOTA	3561	CD1		484	20.271		17.445	1.00	0.00	3A7
ATOM	3562	CD2	LEU	484	19.140	-13.413	18.970	1.00	0.00	3A7
ATOM	3563	С	LEU	484	15.345	-11.234	17.861	1.00	0.00	3A7
ATOM	3564	0	LEU	484	14.779		16.981	1.00	0.00	3A7
		N			15.149		19.142	1.00	0.00	3A7
ATOM	3565		THR	485						
ATOM	3566	CA	THR	485	14.449	-9.702	19.526	1.00	0.00	3A7
ATOM	3567	СB	THR	485	13.528	-9.902	20.697	1.00	0.00	3A7
ATOM	3568	OG1	THR	485	12.643	-10.981	20.430	1.00	0.00	3A7
ATOM	3569	CG2	THR	485	12.694	-8.634	20.978	1.00	0.00	3A7
ATOM	3570	c	THR	485	15.542	-8.739	19.870	1.00	0.00	3A7
								1.00	0.00	3A7
MOTA	3571	0	THR	485	16.525	-9.095	20.514			
ATOM	3572	N	GLU	486	15.407	-7.491	19.395	1.00	0.00	3A7
ATOM	3573	CA	GLU	486	16.478	-6.537	19.402	1.00	0.00	3A7
ATOM	3574	CB	GLU	486	16.229	-5.476	18.329	1.00	0.00	3A7
ATOM	3575	CG	GLU	486	16.097	-6.056	16.918	1.00	0.00	3A7
ATOM	3576	CD	GLU	486	16.045	-4.920	15.900	1.00	0.00	3A7
										3A7
MOTA	3577		GLU	486	15.044	-4.847	15.140	1.00	0.00	
ATOM	3578	OE2	GLU	486	17.014	-4.115	15.863	1.00	0.00	3A7
ATOM	3579	С	GLU	486	16.763	-5.904	20.729	1.00	0.00	3A7
ATOM	3580	0	GLU	486	17.821	-6.121	21.297	1.00	0.00	3A7
ATOM	3581	N	LYS	487	15.871	-5.074	21.275	1.00	0.00	3A7
ATOM	3582	CA	LYS	487	16.181	-4.394	22.523	1.00	0.00	3A7
										3A7
ATOM	3583	СВ	LYS	487	16.681	-2.935	22.345	1.00	0.00	
ATOM	3584	CG	LYS	487	18.078	-2.831	21.710	1.00	0.00	3A7
MOTA	3585	CD	LYS	487	18.582	-1.386	21.553	1.00	0.00	3A7
ATOM	3586	CE	LYS	487	17.737	-0.521	20.606	1.00	0.00	3 A7
ATOM	3587	NZ	LYS	487	17.683	-1.111	19.249	1.00	0.00	3A7
ATOM	3588	c	LYS	487	14.847	-4.380	23.208	1.00	0.00	3A7
						-3.436	22.965	1.00	0.00	3A7
ATOM	3589	0	LYS	487	14.110					
ATOM	3590	N	PRO	488	14.469	-5.369	24.036	1.00	0.00	3A7
ATOM	3591	CA	PRO	488	13.160	~5.418	24.666	1.00	0.00	3A7
ATOM	3592	CD.	PRO	488	15.099	-6.687	23.995	1.00	0.00	3A7
ATOM	3593	СВ	PRO	488	12.772	-6.900	24.541	1.00	0.00	3A7
ATOM	3594	CG	PRO	488	14.103	-7.653	24.646	1.00	0.00	3A7
ATOM	3595	c	PRO	488	13.285	-4.931	26.063	1.00	0.00	3A7
								1.00	0.00	3A7
ATOM	3596	0	PRO	488	14.207	-5.350	26.760			
ATOM	3597	N	ILE	489	12.369	-4.042	26.506	1.00	0.00	3A7
ATOM	3598	CA	ILE	489	12.431	-3.564	27.858	1.00	0.00	3A7
ATOM	3599	CB	ILE	489	12.824	-2.096	28.021	1.00	0.00	3A7
ATOM	3600	CG2	ILE	489	14.258	-1.923	27.475	1.00	0.00	3A7
ATOM	3601	CG1		489	11.831	-1.092	27.392	1.00	0.00	3A7
	3602	CD	ILE	489	12.182	0.356	27.747	1.00	0.00	3A7
ATOM										3A7
MOTA	3603	С	ILE	489	11.136	-3.837	28.577	1.00	0.00	
ATOM	3604	0	ILE	489	10.052	-3.733	28.009	1.00	0.00	3A7
ATOM	3605	N.	VAL	490	11.230	-4.209	29.878	1.00	0.00	. 3A7
ATOM	3606	CA	VAL	490	10.101	-4.648	30.674	1.00	0.00	3A7
ATOM	3607	СВ	VAL	490	9.925	-6.155	30.572	1.00	0.00	3A7
ATOM	3608		VAL	490	9.245	-6.911	31.734	1.00	0.00	3A7
					9.143	-6.483	29.279	1.00	0.00	3A7
ATOM	3609		VAL	490						
MOTA	3610	С	VAL	490	10.398	-4.303	32.085	1.00	0.00	3A7
MOTA	3611	0	VAL	490	11.537	-4.064	32.455	1.00	0.00	3A7
ATOM	3612	N	LEU	491	9.344	-4.289	32.927	1.00	0.00	3A7
ATOM	3613	CA	LEU	491	9.438	-4.005	34.328	1.00	0.00	3A7
MOTA	3614	СВ	LEU	491	8.379	-2.956	34.702	1.00	0.00	3A7
ATOM	3615	CG	LEU	491	8.991	-1.575	35.041	1.00	0.00	3A7
ATOM	3616		LEU	491	7.898	-0.495	35.142	1.00	0.00	3A7
MOTA	3617	CD2	LEU	491	9.848	-1.615	36.322	1.00	0.00	3A7
ATOM	3618	С	LEU	491	9.183	-5.273	35.064	1.00	0.00	3A7
ATOM	3619	0	LEU	491	8.303	-6.043	34.680	1.00	0.00	3A7
ATOM	3620	N	LYS	492	9.934	-5.530	36.165		0.00	3A7
ATOM	3621	CA	LYS	492	9.855		36.930	1.00	0.00	3A7
							37.203		0.00	3A7
ATOM	3622	CB	LYS	492	11.254					
ATOM	3623	CG	LYS	492	12.184		38.201	1.00	0.00	3A7
MOTA	3624	CD	LYS	492	12.735		37.743		0.00	3A7
ATOM	3625	CE	LYS	492	12.568	-4.191	38.784	1.00	0.00	3A7
ATOM	3626	NZ	LYS	492	11.143	-3.831	38.925	1.00	0.00	3A7
ATOM	3627	C	LYS	492	9.148		38.247		0.00	3A7
ATOM	3628	ŏ	LYS	492	9.344					3A7
71011	3020	J			2.544	, . 2))	55.150	2.50		~ ,

ATOM	3629	N	ALA	493	8.315	-5.466	38.338	1.00	0.00	3A7
ATOM	3630	CA	ALA	493	7.783	-4.923	39.576	1.00	0.00	3A7
ATOM	3631	СВ	ALA	493	7.164	-3.529	39.347	1.00	0.00	3A7
ATOM	3632	c	ALA	493	6.735	-5.798	40.223	1.00	0.00	3A7
ATOM	3633	ŏ	ALA	493	5.607	-5.896	39.745	1.00	0.00	3A7
MOTA	3634	N	GLU	494	7.121	-6.449	41.348	1.00	0.00	3A7
				494			42.081	1.00	0.00	3A7
ATOM	3635	CA	GLU		6.270	-7.353		1.00	0.00	3A7
ATOM	3636	СВ	GLU	494	6.221	-8.771	41.447			3A7 3A7
ATOM	3637	CG	GLU	494	5.073	-9.691	41.921	1.00	0.00	
ATOM	3638	CD	GLU	494		-10.327	43.282	1.00	0.00	3A7
ATOM	3639		GLU	494		-10.984	43.425	1.00	0.00	3A7
ATOM	3640	OE2	GLU	494	4.495	-10.171	44.193	1.00	0.00	3A7
ATOM	3641	С	GLU	494	6.833	-7.451	43.468	1.00	0.00	3A7
ATOM	3642	0	GLU	494	6.097	-7.692	44.424	1.00	0.00	3A7
MOTA	3643	N	SER	495	8.180	-7.291	43.592	1.00	0.00	3A7
ATOM	3644	CA	SER	495	9.005	-7.634	44.741	1.00	0.00	3A7
ATOM	3645	СВ	SER	495	10.488	-7.267	44.500	1.00	0.00	3A7
ATOM	3646	OG	SER	495	10.963	-7.890	43.315	1.00	0.00	3A7
ATOM	3647	С	SER	495	8.584	-6.990	46.046	1.00	0.00	3A7
ATOM	3648	ŏ	SER	495	8.318	-5.791	46.117	1.00	0.00	3A7
ATOM	3649	N	ARG	496	8.506	-7.831	47.102	1.00	0.00	3A7
MOTA	3650	CA	ARG	496	8.050	-7.468	48.419	1.00	0.00	3A7
ATOM	3651	CB	ARG	496	6.781	-8.270	48.810	1.00	0.00	3A7
					6.173	-7.918	50.178	1.00	0.00	3A7
ATOM	3652	CG	ARG	496		-8.715	50.471	1.00	0.00	3A7
ATOM	3653	CD	ARG	496	4.896				0.00	3A7
ATOM	3654	NE	ARG	496	4.413	-8.345	51.841	1.00		3A7 3A7
MOTA	3655	CZ	ARG	496	3.354	-8.981	52.430	1.00	0.00	
ATOM	3656		ARG	496	2.955	-8.609	53.681	1.00	0.00	3A7
ATOM	3657		ARG	496	2.696	-9.982	51.778	1.00	0.00	3A7
ATOM	3658	С	λRG	496	9.179	-7.785	49.356	1.00	0.00	3A7
ATOM	3659	0	ARG	496	9.927	-8.738	49.139	1.00	0.00	3A7
ATOM	3660	N	ASP	497	9.312	-6.984	50.445	1.00	0.00	3A7
ATOM	3661	CA	ASP	497	10.298	-7.171	51.489	1.00	0.00	3A7
MOTA	3662	СВ	ASP	497	10.821	-5.830	52.089	1.00	0.00	3A7
MOTA	3663	CG	ASP	497	9.707	-4.881	52.551	1.00	0.00	3A7
MOTA	3664	OD1	λSP	497	8.940	-4.387	51.682	1.00	0.00	3A7
ATOM	3665	OD2	ASP	497	9.625	-4.629	53.783	1.00	0.00	3A7
ATOM	3666	С	ASP	497	9.711	-8.068	52.560	1.00	0.00	3A7
ATOM	3667	0	ASP	497	8.985	-7.622	53.447	1.00	0.00	3A7
ATOM	3668	N	GLU	498	10.021	-9.384	52.458	1.00	0.00	3A7
ATOM	3669	CA	GLU	498		-10.423	53.314	1.00	0.00	3A7
ATOM	3670	СВ	GLU	498		-11.610	52.501	1.00	0.00	3A7
ATOM	3671	CG	GLU	498		-11.185	51.557	1.00	0.00	3A7
ATOM	3672	CD	GLU	498		-12.413	50.822	1.00	0.00	3A7
ATOM	3673		GLU	498		-12.728	50.989	1.00	0.00	3A7
ATOM	3674		GLU	498		-13.049	50.081	1.00	0.00	3A7
	3675		GLU			-10.918	54.195	1.00	0.00	3A7
MOTA		C		498			54.157	1.00	0.00	3A7
MOTA	3676	0	GLU	498		-10.403			0.00	3A7
MOTA	3677	N	THR	499		-11.961	55.010	1.00		3A7
ATOM	3678	CA	THR	499		-12.606	55.905	1.00	0.00	3A7
ATOM	3679	СВ	THR	499		-12.970	57.245	1.00	0.00	
MOTA	3680	OG1		499		-13.726	57.084	1.00	0.00	3A7
MOTA	3681		THR	499		-11.664	57.998	1.00	0.00	3A7
MOTA	3682	С	THR	499		-13.836	55.217	1.00	0.00	3A7
ATOM	3683	0	THR	499		-14.244	54.163	1.00	0.00	3A7
MOTA	3684	N	VAL	500	12.842	-14.455	55.826	1.00	0.00	3A7
MOTA	3685	CA	VAL	500	13.521	-15.621	55.300	1.00	0.00	3A7
MOTA	3686	CB	VAL	500	15.021	-15.588	55.594	1.00	0.00	3A7
MOTA	3687	CG1	VAL	500	15.312	-15.508	57.109	1.00	0.00	3A7
ATOM	3688	CG2	VAL	500	15.739	-16.768	54.903	1.00	0.00	3A7
ATOM	3689	С	VAL	500	12.857	-16.864	55.847	1.00	0.00	3A7
ATOM	3690	ō	VAL	500		-16.984	57.047	1.00	0.00	3A7
ATOM	3691	N	SER			-17.816	54.939	1.00	0.00	3A7
ATOM	3692	CA	SER			-19.059	55.286		0.00	3A7
ATOM	3693	СВ	SER			-18.950	55.320		0.00	3A7
MOTA	3694	OG	SER			-20.142	55.806		0.00	3A7
ATOM	3695	c	SER			-20.035	54.235		0.00	3A7
ATOM	3696	õ	SER	_		-21.094	54.550		0.00	3A7
ATOM	3697	Ŋ				-19.677	52.947		0.00	3A7
			GLY			-20.464	51.805		0.00	3A7
ATOM	3698	CA	GLY							3A7
MOTA	3699	C	GLY			-19.693	51.074			3A7
MOTA	3700	0	GLY	502	13.335	-18.585	50.602	1.00	0.00	JA1

MOTA	3701	N	ALA	503	14.804	-20.283	50.980	1.00	0.00	3A7
ATOM	3702	CA	ALA	503	15.970	-19.715	50.338	1.00	0.00	3A7
ATOM	3703	СВ	ALA	503	15.775	-19.401	48.838	1.00	0.00	3A7
ATOM	3704	С	ALA	503	16.423	-18.443	51.073	1.00	0.00	3A7
ATOM	3705	OT1	ALA	503	17.016	-18.589	52.175	1.00	0.00	3A7
ATOM	3706	OT2	ALA	503	16.167	-17.323	50.557	1.00	0.00	3A7
TER	3707		ALA	503						
HETATM	3708	FE	HEM	600	19.802	-26.909	18.195	1.00	0.00	HEM
HETATM		NA	HEM	600	19.117	-26.973	16.343	1.00	0.00	HEM
HETATM	3710	NB	HEM	600	18.291	-25.763	18.746	1.00	0.00	HEM
HETATM	3711	NC	HEM	600	20.542	-26.830	20.017	1.00	0.00	HEM
HETATM	3712	ND	HEM	600	21.332	-28.034	17.616	1.00	0.00	HEM
HETATM	3713	ClA	HEM	600	19.627	-27.653	15.248	1.00	0.00	HEM
HETATM			HEM	600		-27.461	14.072	1.00	0.00	HEM
HETATM	3715		HEM	600		-26.605	14.439	1.00	0.00	HEM
HETATM			HEM	600		-26.338	15.849	1.00	0.00	HEM
HETATM	3717	ClB	HEM	600	17.258	-25.288	17.964	1.00	0.00	HEM
HETATM	3718	C2B	HEM	600		-24.465	18.724	1.00	0.00	HEM
HETATM			HEM	600		-24.471	20.029	1.00	0.00	HEM
HETATM			HEM	600		-25.267	20.000	1.00	0.00	HEM
HETATM			HEM	600		-26.220	21.122	1.00	0.00	HEM
HETATM			HEM	600		-26.398	22.303	1.00	0.00	HEM
HETATM			HEM	600		-27.105	21.896	1.00	0.00	HEM
HETATM			HEM	600		-27.359	20.473	1.00	0.00	HEM
HETATM			HEM	600		-28.419	18.358	1.00	0.00	HEM
HETATM			HEM	600		-29.229	17.581	1.00	0.00	HEM
HETATM			HEM	600		-29.362	16.350	1.00	0.00	HEM
HETATM			HEM	600		-28.591	16.366	1.00	0.00	HEM
HETATM			HEM	600		-28.392	15.257	1.00	0.00	HEM
HETATM			HEM	600		-25.582	16.615	1.00	0.00	HEM
HETATM			HEM	600		-25.488	21.097	1.00	0.00	HEM
HETATM			HEM	600		-28.078	19.676	1.00	0.00	HEM
HETATM			HEM	600		-26.027	13.539	1.00	0.00	HEM
HETATM			HEM	600		-28.152	12.738	1.00	0.00	HEM
HETATM			HEM	600		-27.341	11.731	1.00	0.00	HEM
HETATM			HEM	600		-28.082	10.424		0.00	HEM
HETATM	3737	Ola	HEM	600	18,997	-28.897	10.031	1.00	0.00	HEM
HETATM			HEM	600		-27.812	9.777	1.00	0.00	HEM
HETATM			HEM	600		-23.749	18.107	1.00	0.00	HEM
HETATM			HEM	600		-23.874	21.208	1.00	0.00	HEM
HETATM			HEM	600		-23.138	21.387	1.00	0.00	HEM
HETATM	3742	CMC	HEM	600	20.479	-25.906	23.689	1.00	0.00	HEM
HETATM	3743		HEM	600		-27.556	22.589	1.00	0.00	HEM
HETATM	3744	CBC	HEM	600	23.305	-27.610	23.914	1.00	0.00	HEM
HETATM			HEM	600		-29.779	18.033	1.00	0.00	HEM
HETATM	3746	CAD	HEM	600	23.358	-30.183	15.203	1.00	0.00	HEM
HETATM			HEM	600		-31.591	15.127	1.00	0.00	HEM
HETATM			HEM	600		-32.470	14.027	1.00	0.00	HEM
HETATM	3749		HEM	600 .	23.719	-33.625	14.347	1.00	0.00	HEM
HETATM	3750	02D	HEM	600		-32.020	12.856	1.00	0.00	HEM
END										

Sequences:

SEQ ID N°1: P450 Nor, crystal structure 1rom

SEQ ID N°2: P450 Ery F, crystal structure 10xa

SEQ ID N°3: P450 Terp, crystal structure 1cpt

5 SEQ ID N°4: P450 Cam, crystal structure 3cpp

SEQ ID N°5: P450 BM3, crystal structure 2hpd

The sequence corresponding to the PDB structure includes 471 residues. For more clarity in Figure 1, the last 12 residues have been omitted, the C-terminal part having no equivalent counterpart in the other structures aligned.

10 SEQ ID N°6: P450 2C5, crystal structure 1dt6

Cyp2C5 from Oryctolagus cuniculus (Rabbit), with membrane spanning residues 3-21 deleted and a 4 residue histidine tag at the C-Terminus containing additional internal mutations.

SEQ ID N°7: P450 2C5 rabbit

15 Sequence corresponding to the non-mutated CYP 2C5 gene from Oryctolagus cuniculus (Rabbit), consistently with SwissProt CPC5 RABIT P00179.

SEQ ID N° 8: CYP51, crystal structure 1e9x

Cyp51 from Mycobacterium tuberculosis, with a 4 residue histidine tag at the C-Terminus.

20 SEQ ID N°9: CYP3A1 rat

SEQ ID N°10: CYP3A3 human

Cytochrome P-450, a possible variant of CYP3A4, inducible by glucocorticoids in human liver.

SEQ ID N°11: CYP3A4 human

Numbering starts at Ala 1 (first residue Met is not included, consistently with SwissProt CP34 HUMAN P08684)

SEQ ID N°12: CYP3A5 human

SEQ ID N°13: CYP3A43 human

SEQ ID N°14: CYP3A6 rabbit

30 SEQ ID N°15: CYP3A7 human

SEQ ID N°16: CYP3A12 dog

SEQ ID N°17: CYP3A29 pig

SEQ ID N°18: CYP3A13 mouse

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Figure 1: Structure-based alignment of human cytochromes P450 3A3, 3A4, 3A5, 3A7 and 3A43 and of selected mammalian P450 3A isozymes, with bacterial P450 crystal template structures and rabbit P450 2C5 crystal template structure.

- Sequence numbering is indicated for each enzyme of the structural template and for the human 3A4 and 3A7 isozymes, as examples given in the present invention. This alignment is first based on the structural alignment of bacterial P450s and rabbit P450 2C5 derived from GOK analysis. Human P450 3A sequences were then aligned with in-house tools that locates the CSBs on the target sequence. The alignment shown outside the CSBs is not relevant, as there is no structural information available in these regions. The CSB sequences are indicated by bold uppercase characters and are highlighted in grey. Amino acids strictly conserved between CYP3A and 2C5, or between CYP3A and all the sequences of crystal structures, are highlighted in black.
- Figure 2: Ramachandran plot of a lowest energy model of CYP3A4 produced by DYANA-XPLOR calculations from the six-template structural alignement. Figure 3: view of one optimized CYP3A4 model. This figure can be replaced by the whole set of coordinates file of table 3 in the PDB format.
 - Figure 4: final position of testosterone into the CYP3A4 and CYP3A7 active sites after soft-restrained dynamics docking. The active sites are characterized by six Substrates Recognition Sites (SRS, after Gotoh 1989, in bold) associated to fragments of secondary element structures (in italic).

Panel 4A In CYP3A4 active site, the docked testosterone molecule is oriented so that the A steroid cycle (carrying in position 3 a carbonyl function with an oxygen atom symbolized by a large ball) is close to the heminic iron. This supports the propensity of CYP3A4 to metabolize testosterone in 6 β position as indicated by the black solid arrow.

Panel 4B In CYP3A7 active site, the docked testosterone molecule is oriented so that the D steroid cycle (carrying in position 17 a hydroxylic function with an oxygen atom symbolized by a large ball) is close to the heminic iron. This supports the propensity of CYP3A7 to metabolize testosterone in 16 α position as indicated by the black solid arrow

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Figure 5: Energy profile of the soft-restrained dynamics docking of testosterone into CYP3A4 model.

Example 1: Determination of the 3D-structure of P450 3A4.

5 Material

The coordinates of the six P450 crystal structures: P450cam (3cpp), P450terp (1cpt), P450BM-3 (2hpd), P450eryF (1oxa), P450 nor (1rom) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank. The structural alignment and the conserved regions determination were realized using the GOK software (Jean et al. 1997) running on an Octane Silicon-Graphics workstation. Structures were built using the DYANA (Güntert et al. 1997), and X-PLOR softwares (Brünger 1992). Docking studies were performed with SYBYL 6.6 (Tripos Inc.) and TRIPOS force field. The structures were analyzed using Procheck-NMR (Laskowski et al. 1993) and visualized under SYBYL 6.6 (Tripos Inc.).

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Common Structural Blocks (CSB) determination.

The first key point of this homology modeling study is the identification of the structural elements (hereafter designed as CSBs for Common Structural Blocks) conserved among the family of cytochromes P450 of known 3D structures, and the localization of these elements in the target sequence. These two tasks are performed using the GOK software (Jean et al. 1997), and are well described in a forthcoming article (Minoletti et al., Proteins, Structure, Function and Genetics, 2002). In brief, the basic idea of CSB identification by GOK is to use an internal coordinate representation – (α, τ) in our case (another representation of ϕ , ψ and ω angles) – and to search for fragments in the six-template proteins having similar local trajectories in the internal coordinate space. GOK provides two adjustable parameters (the α -mesh and the α -margin) that define the tolerance on the comparison of the trajectories. These parameters were adjusted recursively to values ranging from 15 to 30° (α -mesh) and 1 to 3 (α -margin in mesh units). The evaluation of the quality of the match was measured using two multiple-way rmsd calculated in the cartesian coordinates space: mp-rms (the mean of all pairwise rms deviations) and s-rms (the mean of the deviations calculated with respect to a mean structure obtained from the average internal coordinates). For the different CSBs,

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mp-rms value ranged between 0.3 and 4.9 Å in average, and s-rms between 0.04 and 2.4 Å.

CYP3A4 sequence alignment and evaluation of the profile

5 The multiple sequence alignment derived from the CSB identification was then used to build a similarity profile. The profile is defined as a position-specific scoring table created from aligned gap-free segments such as CSBs (Jean et al. 1997). The alignment then consists in a search of the best match (as per the best score) between a CSB of sequences defined structurally (i.e. independently of the nature of the aligned residues) and several other sequences that are well-aligned and exhibit a high sequence identity. In the P450 3A subfamily, many proteins exhibit high sequence identity. We extended our profile search program to take this information into account, i.e. to align the profile with a pre-defined multiple alignment of the cytochromes P450 3A subfamily members sequences (Gotoh 1992; Nelson et al. 1996). The similarity score was calculated using BLOSUM62 matrix (Henikoff and Henikoff 1992). The in-house tool SmartConsAlign (Atelier de Bioinformatique, Université Paris VI) described in Jean et al. 1997, allows to move the consensus matrix along the multiple sequence alignment of P450 3A family, and computes for each position a score of similarity. The best alignment found of 20 CYP3A4 on CSBs is shown in Figure 1.

Once the alignment is completed, the 3D model rebuilding process can incorporate the atom Cartesian coordinates of the template structures only for amino acids located in structurally conserved regions (*i.e.* the CSBs). The coordinates of any of the template structures can be used for determining the final template. In each CSB, amino acid positions have been renumbered according to the sequence of human P450 3A4. At a given position, when residues are identical between all the template structures and the target sequence, the 3D coordinates of the reference residues are purely assigned to the modeled (target) residue. When residues differ, only the coordinates of the backbone atoms are assigned ($C\alpha$), and sometimes $C\beta$ when they exist. Side chains are rebuilt from libraries giving the most probable rotamers for each amino acid (see below). In some cases, it was possible to superimpose the positions of carbon atoms of lateral chains up to ranks γ and δ along the sidechain, thus explicitly defining a unique rotamer.

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For amino acids located outside the CSBs (structurally variable zones that include generally loops), the rebuilding is more complex, and can be done only after rebuilding of structurally conserved zones. In the multiple structural alignment (Figure 1), the regions separating the CSBs bring no structural information at all.

5 Short loops are rebuilt entirely, since solutions of acceptable geometry for atoms are in limited number, *i.e.* the lowest energy drives the selection of the good geometry. For longer segments, various structures are provided by the constrained minimization runs, and a manual selection is operated.

10 Constraints derivation and rebuilding

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A strategy inspired of the techniques commonly used to built structures from NMR data (Patard et al. 1996) is applied. The main idea is to express all available information issued from the comparison of the templates in term of geometrical constraints (distances and angles). Each constraint will be defined as an interval (for a given pair of atoms, this is the average of the six atom-atom distances found in the template structures +/- the standard deviation), similarly to the strategy developed by Havel and Snow (Havel and Snow 1991). However, the number of constraints corresponding to all atom-atom distances, for example, would be prohibitive for a protein of the size of the P450 (around 1,000,000 inter-residual distances if we consider 250 conserved residues and an average of four atoms per residues). Previous NMR studies (Patard et al. 1996) have shown that local constraints are sufficient to allow a correct reconstruction of a structure. This reduces drastically the number of constraints needed, and increases the flexibility of the model. In addition, similarly to what is done in protein structure determination by NMR, we can build a family of structures instead of a single model. This allows an easier analysis of the well or less well-predicted regions. This is also an advantage for the analysis of the side-chain positions, particularly in prevision of a substrate docking study. Finally, the loops are passively reconstructed with the rest of the structure. The only specific information we have introduced in variable regions was to guide all their residues to an allowed region of the Ramachandran diagram. Indeed, analysis of well-defined structures shows that nearly all residues, including those of the loops, should belong to an allowed region. The lower the proportion of residues

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found outside the allowed Ramachandran regions, the better the structure is. This criterion of quality has been applied to derive the model described herein.

Accordingly, we retained for model rebuilding all the distance and angle intervals corresponding to the following principles:

- all distances for which the lower boundary was less than 8 Å. This cutoff is totally sufficient to ensure, at least, the formation of the local structure elements. Such a cutoff is relatively high and thus costly in terms of size of constraints file, but proved necessary to ensure good results for the P450s. This may be due to the fact that P450 enzymes are mostly formed of α-helices, the average distance between two helices being larger than between two adjacent β-strands. In addition, the percentage of residues located outside CSBs is rather high in the structural alignment of P450s, and a better convergence can be obtained only at the expense of a high number of rebuilding distance constraints.
 - all the distances involving at least one side-chain atom, to preserve the spatial arrangement between CSBs
 - finally, all the distances involving atoms of the heme group, to fix as much as possible the neighborhood of the iron atom.

The total number of distance constraints was, in these conditions, equal to 58506. Similarly, angular constraints were calculated in each building block. A CSB is indeed defined as a conserved trajectory in the φ, ψ coordinates space (or α, τ). Thus, dihedral angles φ and ψ of all residues located in CSBs can be defined as constraints, given by the average values of corresponding φ, ψ angles in the six templates +/- the standard deviation. To these backbone dihedral angles, can be added the side chains torsion angles χ_1 , χ_2 whenever possible, as determined by the rotamer selection. The total number of dihedral angle constraints was, in these conditions, equal to 761.

Rotamer selection

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In proteins, the preferential orientation of the side chain (60°, -60°, 180°) depends on the local conformation of the residue, and thus on the nature of the secondary structure in which the residue is involved. According to the rotamer library built by Karplus and coll. (Dunbrack and Karplus 1993), to a given (φ, ψ) couple in the

Ramachandran diagram can be associated a specific rotamer for each type of residue. These tables have been used to determine the most probable rotamer for each residue located in CSB, except when there are conserved atoms in the side chain that assign unambiguously a rotamer (χ_1, χ_2) . The selected (χ_1, χ_2) couples were included in the above-mentioned set of angle 761 dihedral constraints.

Structure calculation and optimization

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We used a procedure similar to structure calculation starting from NMR constraints. A first set of structures was calculated using the DYANA software (Güntert et al. 1997) and the 58506 distance and 761 angular constraints. Families of structures are generated. The energy of each structure is minimized with the procedure vtfmin in DYANA.

Due to the size and the amount of loops in the molecule, some structures presented topological defects and were discarded. The others were further optimized by using the X-PLOR software. A set of constraints was added at this stage in order to guide the loop residues to the nearest allowed region in the Ramachandran diagram. The topology and parameter files of CHARMM22 were used. The electrostatic term was turned off.

The DYANA software is unable to deal with disconnected objects. A new residue type was, thus, added to the standard amino acid library to take into account the the presence of the heme. This residue was obtained by combining the heme to a cysteine and was inserted at position 441 in the sequence of the protein (Figure 1).

Description of the CYP3A4 Model

We rebuilt a model of the protein depleted of its first 50 residues (N-terminal domain). This segment is highly hydrophobic, and supposed to form the anchor of the protein in the membrane. There is no structural information about this putative transmembrane domain, and this segment was thus not incorporated into the modeling process, and in the final model. Such a "free" segment (with no constraints) would perturbate the convergence of computation or the stability of the whole rebuilt structure.

The quality of the various structures optimized under XPLOR was checked for the stereochemical quality (backbone and side chain conformation) by PROCHECK

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(Laskowski et al. 1993). The Ramachadran plot shows that our six-template approach generated converging models, possessing the same fold. The lowest energy models had 73% of their non-glycine and non-proline residues with φ, ψ conformation in the most favoured regions of the Ramachandran plot (core region), 20% in additional allowed regions, and 5% in the generously allowed regions. Only 2.3% (9 residues) had their φ, ψ conformation in disallowed regions (Figure 2). The total number of residues in the model is 452; which 399 are non-glycine and non-proline residues, and number of residues in the native sequence is 502.

When compared to the CYP2C5 crystal structure, it can be noticed that the CYP3A4 model exhibits a good 3D similarity in the global fold than expected, since this structure counts only for one in the six-template approach. This proves that in this approach, there is no "averaging" effect, *i.e.* the mammalian structure had a decisive influence over the five bacterial (and fungus) templates. Our final fold of CYP3A4 is very consistent with a mammalian one, despite the fact that it has been rebuilt by using the structural information contained in non-mammalian cytochromes P450.

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The active site is delimited by the six substrate recognition sites (SRS) that have been first identified and described by Gotoh (Gotoh 1992) from the unique structure available in the early 1990s (P450_{cam}), and that are today commonly accepted for depicting substrate recognition by various cytochromes P450 (especially from the family 2, but extended to other P450 families). These sites are associated with the active site and are located in the less conserved regions of the CYPs, thus possibly accounting for the various substrate specificity among P450s. When comparing our various optimized structures, it is found that SRS1 (100-125, includes helix B), SRS 2 (205-218, includes C-terminus of helix F), and SRS3 (237-249, includes Nterminus part of helix G) are located in less-defined regions, with significant variability in spatial position (flexibility). These regions correspond also to parts of the sequence that are less well-aligned. At the opposite, the SRS4 (295-320, central part of helix I), SRS5 (363-380, C-term of helix K and β-sheet β1-4) and SRS6 (470-490, β -sheets β 4-1 and β 4-2) are well-defined fragments of the structures. SRS4 and SRS5 segments in particular are correlated to regions in the sequence that are unequivocally aligned.

The only model structure of CYP3A4 that has been described in the literature and that we can handle for structural comparison, is that of Szklarz and Halpert, derived from a multiple-template approach (four-bacterial template) (Szklarz and Halpert 1997). Roughly, the same secondary structures are identified, but we found 5 divergences in SRS location between their model and those derived from the present approach. SRS4 and SRS5 match well, but SRS2 is shifted (divergence in the position of helix F along the sequence), while SRS1 (helix B'), SRS3 (helix G) and SRS6 (sheet \$\beta 4\$) are more notably displaced. The loops connecting the secondary structures of these SRS significantly disagree. These differences are likely to issue from a wrong alignment with the crystal P450 structures in the model of Szklarz and Halpert.

Example 2: Determination of the 3D-structure of P450 3A7.

The model rebuilding of CYP3A7 was performed according to the techniques described above in example 1 for CYP3A4, except that we used a restrained set of four-template structures, still including the mammalian CYP2C5, in order to test the robustness of the modeling approach. Below are pointed out only the differences in input data and the results relevant to CYP3A7.

Material 20

The coordinates of the four P450 crystal structures: P450BM-3 (2hpd), P450eryF (10xa), P450 51-like from Mycobacterium tuberculosis (1e9x) and P450 2C5 (1dt6) were retrieved from the Brookhaven Protein data bank and used as initial template for GOK analysis.

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Common Structural Blocks (CSB) determination.

The GOK parameters were adjusted recursively to values ranging from 10 to 30° $(\alpha$ -mesh) and 1 to 3 $(\alpha$ -margin in mesh units). Occasionally, the α -mesh value was pushed up to 60° to refine some local structured loops (DE loop, HI loop) or short helices (such as J'). 27 CSBs have been identified. New CSBs were detected: the block 7* (between blocks 6 and 7A), the block 7B* (between 7B and 8) and the block 7C (between 7B* and 8). For the different CSBs, mp-rms value ranged between 0.12 and 4.57 Å in average.

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The best alignment found of CYP3A7 on CSBs is shown in Figure 1. On the 459 residues comprised in the model structure (the protein was rebuilt depleted of its first 44 residues from the N-terminal domain), 337 residues were found located in CSBs, i.e. 73% of residues belong to structurally conserved regions of the four-template set.

Constraints derivation and rebuilding

With a larger cutoff (12 Å), we obtained around 73000 distance constraints, and 900 dihedral constraints.

The residue covalently linked to the heme group is at position 442 in the sequence of the protein (Figure 1).

Description of the CYP3A7 model

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The four-template approach generated converging models, possessing the same fold. The PROCHECK analysis for structure quality assessment for the lowest energy models showed 74.4% of their non-glycine and non-proline residues with φ , ψ conformation in the most favoured regions of the Ramachandran plot (core region), 18.2% in additional allowed regions, and 4.7% in the generously allowed regions. 2.7% (11 residues) had their φ , ψ conformation in disallowed regions. The total number of residues in the model is 459; which 407 are non-glycine and non-proline residues, and number of residues in the native sequence is 503.

A closer inspection of the structure, and after the results of dynamics docking experiments (see below), revealed that several hydrogen bonds can hinder the main access to the active site. Thus, key residues that are likely to be involved in the recognition and admission of the substrate are Q79; F102; R105; R106; F108; F248; F304 and E374, and additionally C98 and C377 (Figure 4B). More specifically, R105, R106, Q79 and E374 can establish mutual hydrogen bonds in one of the access channels, and are thus involved in the access of the substrate towards the active site.

Example 3: Docking Strategy

Our aim in this example was to obtain the different positions of the known substrates of CYP3A in the active site, consistent with the oxidation sites and

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biochemical differences among the CYP3A isoforms. Considering the fact that the heme-binding site is deeply buried in the protein structure, and thus the selection and the pathway of the substrates within the enzyme structure are strongly dependent on the various possibilities of structure opening, we implemented a special approach more appropriate to flexible structures, hereafter referred as "restrained dynamics docking" or "soft-restrained dynamics docking". This technique employs constrained molecular dynamics simulations, where the only constraints are heme-substrate distances. The successive steps are:

10 Conversion of the PDB XPLOR file in PDB for SYBYL file

The optimized structures with XPLOR (PDB format) are visualized with the SYBYL 6.6 software (Tripos Inc.), which implies a conversion of the file (atoms types correction) so as to make it compatible and exploitable in the constrained dynamics which will be performed with SYBYL.

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Stabilization of the P450 3A4 model generated under XPLOR

Then, we do agregate N°1 (in the meaning of SYBYL) with all the $NC_{\alpha}CO$ atoms of the peptide backbone of the protein. The structure is relaxed with a dynamic of 10ns at 100K followed by a minimization of 100 steps. Agregate N°1 is then deleted.

We do agregate N°2 constituted of the protein C_{α} only. The protein relaxation is reiterated with a dynamic of 10 ns at 100K and a minimization of 100 steps. Agregate N°2 is then deleted.

The all protein is then relaxed with a first dynamic of 1ns at 100K, followed by a dynamic of 1ns at 200K and a dynamic of 10ns at 300K. We terminate with a minimization of 100 steps.

Restrained dynamics docking of the substrate (example: testosterone)

We do agregate N°3 constituted of all atoms outside a sphere of 20Å around the C_{α} of residues constituting the heart of the B' loop. We also add heminic iron to this aggregate.

The substrate is placed inside the protein, at around 30Å from the heminic iron and next to SRS1 and SRS5 sites. The substrate is placed so that the contraints between

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the heminic iron and the substrate backbone go between SRS1, SRS5 and SRS3. Thus, for testosterone docking, we establish 4 distance contraints (limit below 3Å, above 10Å) between heminic iron and C3, C8, C10 and C13 carbons with a constraint of 2 kcal/Å on the entire structure so as to avoid to favour the approach of one part of the substrate more than the other.

We begin to perform a dynamic without contraints of the entire system at 20 K during 2ns to stabilize the system, then we perform a dynamic under contraints at 20 K during 5ns. We observe that the substrate worms between SRS1, SRS3 et SRS5 to reach a position at the vicinity of heminic iron. We terminate with a dynamic without contraints at 300 K to relax the system and we realize a minimization of 1000 steps.

Results

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We found that the testosterone molecule is positioned at the vicinity of heminic iron in such way that the C6 of testosterone be at 4.9Å of the iron, which is compatible with the hydroxylation of this compound to give 6β -hydroxy-testosterone (Figure 4A).

Minimizations and dynamics with the SYBYL software are performed with the Tripos force field following the parameters: dielectric constant equal to 1 and distance-dependent, minimization method of POWELL, a minimum gradient of 0.05kcal.mol⁻¹.Å⁻¹, electrostatics charges calculated according to the Gasteiger-Hückel method, and a NB cutoff of 8.0Å (non-bond energies). The energetic diagram of dynamic docking of testosterone is shown in **Figure 5**.

25 Interest of this docking strategy:

Most P450 isozymes recognize only one substrate (for specific catalysis in a metabolic pathway), or a very limited number of substrates, all chemically closely related. At the contrary, CYP 3A isozymes are known to recognize a large palette of substrates, and are also capable of multiple binding in the active site, up to three molecules in the vicinity of the heme, according to the model developed by Hosea et al. 2000. Multiple pharmacophoric behavior (Ekins et al. 2003), as well as allosteric or synergistic effects, characterize the members of this P450 subfamily.

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The docking strategy described above can be easily extended to different binding and metabolism scenario.

For example, the docking of two or three testosterone molecules, or of two testosterone molecules and one alpha-naphtoflavone molecule (αNF) can be simulated in the following manner:

- In a first step, a testosterone molecule is dynamically docked under constraints, and then released of its constraints to freely evolve in the active site and find a first bound equilibrium position.
- In a next step, an external testosterone is presented, at the same entrance of the
 protein structure or in the vicinity of another access channel, and then dynamically docked under constraints. The system first evolves under constraints applied to the second molecule, and can be released for a subsequent free MD simulation of the two molecules bound in the active site. One can see the first bound molecule (testosterone or another substrate) to be re-oriented under the effect of the second docking, simulating a situation of cooperativity.
 - Similarly, the second molecule docked can be different from the first bound, e.g. a first testosterone bound to the active site followed by the docking of an αNF molecule, or the reverse situation.
 - One can combine of course the possibilities: for example, two molecules (identical or of different chemical nature) are docked following the two steps above, and then, after stabilization around an equilibrium position, a third molecule is introduced under constraints, and then released from its constraints to let the system evolving towards a favorable energetic conformational state. In this way, two αNF and one testosterone or one αNF and two testosterone can be docked.
- Of course, not only substrates can be docked, but also inhibitors. The docking procedure above can help to measure the potential inhibitory power of a molecule, for example a compound comprising an imidazole group. A first step would include a standard constrained dynamic docking of the potential inhibitor, followed by a free MD simulation (constraints are released when the inhibitor is in the active site), or by a specifically-constrained MD simulation where the imidazole group is confined in the vicinity of the heminic iron by using an additional distance constraint Fe-imidazole. In a following step, a second substrate is dynamically docked under constraints from the exterior, and one can determine in what

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conditions the second molecule can chase the first one from its binding position. The strength of the additional constraint can be a measurement of the inhibitory potential.

Correspondingly, the exit pathway of the metabolites can be explored by simulating the exit of the molecule bound to the active site, using either free MD simulation (if the chemical nature of the transformed molecule allows an energetical instability), or using inverted constraints, *i.e.* soft distance constraints (between an external point and the bound molecule) that help to expel out the metabolite. Additionally, the best exit pathway can be deduced from the most favored energy profiles.

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